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**COMPUTER PROGRAM FOR CALCULATION OF A GAS  
TEMPERATURE PROFILE BY INFRARED EMISSION -  
ABSORPTION SPECTROSCOPY**

by Donald R. Buchele  
Lewis Research Center  
Cleveland, Ohio 44135  
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# COMPUTER PROGRAM FOR CALCULATION OF A GAS TEMPERATURE PROFILE BY INFRARED EMISSION - ABSORPTION SPECTROSCOPY

by Donald R. Buchele

Lewis Research Center

## SUMMARY

A computer program to calculate the temperature profile of a flame or hot gas is presented in detail. Emphasis is on profiles found in jet engine or rocket engine exhaust streams containing  $H_2O$  or  $CO_2$  radiating gases. The temperature profile is assumed axisymmetric with an assumed functional form controlled by two variable parameters. The parameters are calculated using measurements of gas radiation at two wavelengths in the infrared. The program also gives some information on the pressure profile. A method of selection of wavelengths is given that is likely to lead to an accurate determination of the parameters. The program is written in FORTRAN IV language and runs in less than 60 seconds on a Univac 1100 computer.

## INTRODUCTION

Infrared emission and absorption measurements at two or more wavelengths provide a means of determining a gas temperature profile along a path through the gas by using a radiation source and receiver located only at the ends of the path (ref. 1). In the case of a jet engine or rocket engine exhaust stream, the instrumentation may be outside of the stream. The method has been termed the "spectral-scanning method." Practical instruments that permit use of this technique are described in references 1 through 4.

Tests of the method with heated pure gases in a furnace of 60 cm path length (ref. 2), and then with flames over a 22 cm path length

(ref. 3) gave good results. An analysis in reference 5 showed the effect of radiometric errors on the accuracy of the computed profile. The analysis assumed the partial pressure of the radiating gas was a constant over the entire path, with the constant determined from radiometric measurements. More recently, the feasibility of using only emission measurements and an estimated gas composition to determine industrial furnace temperature profiles over a 10-meter path length at atmospheric pressure has been shown (ref. 6).

The computer program presented herein involves an iterative, cyclic computation in which an initial assumed (arbitrary but realistic) temperature profile is altered in shape until the computed emission and absorption that it would yield agree as closely as possible with the actual instrumental measurements of emission and absorption. The procedure requires the use of a large-scale computer. These procedures have been outlined in principle in previous publications; but this report presents an actual program that has been found to produce useful results.

The present work also extends the work of reference 5 by providing greater latitude in the temperature-profile shape that can be treated and by relaxing restrictions on the shape of the associated pressure profile. Thus, whereas previous studies have principally treated profiles with a substantial temperature difference over the optical path, the present study also includes the equally important case of an almost isothermal profile; and whereas the work of reference 5 has assumed constant pressure over the path, the present work allows an additional degree of freedom in the description of the pressure profile.

The program presented provides a means of determining temperature from experimental measurements of emission and absorption at two or more wavelengths. But it also provides a means, before any experiments are performed, of selecting those wavelengths whose use will lead to the best attainable accuracy. This prior selection is very important, because a poor selection of wavelengths may lead to unacceptably high uncertainty in the temperature and may even lead to an erroneous solution of the equations. The existence and avoidance of this incorrect solution for the

temperature profile is demonstrated. Thus, this report provides the potential user with a means of determining whether this method will be sufficiently accurate for his particular application, as well as providing a means of finding the solution if the method is adopted. Symbols are listed in appendix A.

## MATHEMATICAL ANALYSIS

### Method of Determining Temperature and Pressure Profiles

The method is iterative with each iterative step consisting of three principal parts:

1. With current profiles of temperature and pressure, compute the gas radiance and transmittance at each wavelength of measurement.
2. Record the difference between computed and measured gas radiance and transmittance at each wavelength of measurement.
3. Correct the current profiles in (1) to reduce the differences in (2) to zero.

Functional forms of the temperature profile  $T(x)$  and the partial pressure profile  $p(x)$  of the absorbing gas are assumed in advance. The temperature profile is expressed in terms of two unknown parameters, and the pressure profile in terms of one unknown parameter. A minimum of one set of measurements, at each of two wavelengths, is required to yield a solution for the unknown parameters; each set actually involves four radiometric measurements (i. e., four instrument readings). The computational program then determines, from the simultaneous solution of equations containing actual radiometric measurements, the values of these parameters that make computed values of radiance and transmittance equal to measured values.

Additional wavelengths of measurement may improve accuracy; in such case, a least-squares method of solution is employed. The results obtained are the values of the parameters when the "residual", which is the sum of the squares of the differences between measured and computed values of radiance, is a minimum.

The functions used in this program may be modified as desired for a particular application. However, tests during development of the program have shown that it is impractical to characterize the temperature profile by more than two unknown parameters because the accuracy of the solution becomes unacceptably low.

The profiles. - In the present program, the profiles are taken to be axisymmetric, with shapes chosen to resemble the transverse pressure and temperature distributions often found in ducts. The functions are expressed in terms of values of the dependent variable at the axial, or centerline, position (subscript c) and at a wall position (subscript w), and the value of a shape parameter  $\eta_T$  or  $\eta_p$  for temperature or pressure, respectively.

1. When the temperature profile is far from isothermal, it is taken as

$$T(x) = T_c - (T_c - T_w)|y|^{1/\eta_T} \quad (1)$$

where

$$y = (2x/L) - 1 \quad 0 \leq x \leq L$$

It is assumed that  $T_w$  is measured independently. Parameters  $T_c$  and  $\eta_T$  are determined by the computational program. They are then termed the dependent parameters. This family of curves is shown in figure 1(a).

2. When the profile is nearly isothermal, except for a thin boundary layer at each end, the temperature profile is taken as

$$T(x) = T_c - (T_c - T_w^*)|y|^{1/\eta_T} \quad (2a)$$

where

$$y = (2x/L) - 1 \quad x_1 \leq x \leq L - x_1$$



and

$$T(x) = T_w + (T_1 - T_w)z + (mx_1 + T_w - T_1)z(z - 1) \quad 0 \leq z \leq 1 \quad (2b)$$

where

$$z = x/x_1 \quad \text{for } 0 \leq x \leq x_1$$

$$z = (L - x)/x_1 \quad \text{for } L - x_1 \leq x \leq L$$

$$T_1 = T(x_1) = T(L - x_1)$$

$$m = (dT/dx)_{x=x_1} = 2(T_c - T_1)/\left[\eta_T(L - 2x_1)\right]$$

This definition of  $T(x)$  provides continuity of both temperature and temperature gradient at  $x = x_1$  and at  $x = L - x_1$ . This family of curves is shown in figure 1(b). Using this definition,  $\eta_T$  and  $x_1$  are preassigned some reasonable values and the computational program determines  $T_w^*$  and  $T_c$  as the dependent parameters. It is assumed that  $T_w$  is measured independently.

3. The partial pressure profile of each absorbing gas is assumed to be of the form

$$p(x) = p_c - (p_c - p_w)|y|^{1/\eta_p} \quad (3)$$

where

$$y = (2x/L) - 1 \quad 0 \leq x \leq L$$

The profile is shown in figure 1(c). Different initial values may be assumed for parameters  $p_c$ ,  $p_w$ , and  $\eta_p$  for each gas. The choice of the initial values of the parameters may be aided by a computation of the partial pressure of the reaction products. These pressures can be computed for a range of reaction product temperatures and a range of partial pressures

and reactant composition using the computer program of reference 7. From these data a choice for initial values of the pressure parameters can be made. (The program of ref. 7 may be obtained from its authors, on written request, by sending a magnetic tape at least 1200 ft long and by specifying the type of computer. Parts of the program not used in this application may be removed after the program has been transferred from tape to cards.)

Tests during the development of the program for computing temperature and pressure profiles have shown that only one dependent pressure parameter can be determined with acceptable accuracy. This is best done by designating the parameter  $p_{c,1}$  of the principal absorbing gas (subscript 1) as an independent parameter. The wall pressure  $p_{w,1}$  is selected to be directly proportional to the center pressure, and the shape parameter  $n_{p,1}$  is chosen judiciously and held constant. Assumed parameters for all other absorbing gases (subscript  $k$ ) and all nonabsorbing gases (subscript  $j$ ) determine the initial pressure profiles  $[p_k(x)]_0$  and  $[p_j(x)]_0$ .

Next, these profiles are made dependent on the profile  $p_1(x)$ . The absorbing gases initially have profiles that determine ratios  $[p_k(x)/p_1(x)]_0$ . Then, as  $p_1(x)$  is changed by the program, these other profiles are also changed by the linear relation

$$p_1(x)[p_k(x)/p_1(x)]_0 \quad (4)$$

After the absorbing-gas pressure profiles are determined, the non-absorbing-gas pressure profiles  $p_j(x)$  are adjusted to make the sum of all gas pressures equal to the measured static pressure  $p_S$  which is assumed to be independent of  $x$ , so that

$$p_S = \sum_k p_k(x) + \sum_j p_j(x)$$

An additional constraint is to maintain the relative amounts of each non-absorbing gas as given by the initial profiles, that is, in the ratio

$$[p_j(x)/\sum_j p_j(x)]_0$$

Thus the pressures of the nonabsorbing gases are given by

$$p_j(x) = [p_s - \sum_k p_k(x)] [p_j(x)/\sum_j p_j(x)]_0 \quad (5)$$

The residuals. - Initial values of all parameters of the profile functions are tabulated, and the resultant sets of values of gas radiance  $N_L$  and transmittance  $\tau_L$  are computed for two or more wavelengths from radiometric equations. The computed quantities are denoted by  $^c N_L$  and  $^c \tau_L$ . The corresponding measured quantities at the same wavelengths are denoted by  $^m N_L$  and  $^m \tau_L$ . The difference between the computed and measured quantities is called the "residual." The residual for gas radiance may be expressed as a fractional value

$$R_N = (^c N_L - ^m N_L)/^m N_L \quad (6)$$

It is preferable to use gas absorptance  $\alpha_L = 1 - \tau_L$  in place of transmittance  $\tau_L$  for the transmittance residual because  $\alpha_L$  is more nearly proportional to the gas pressure and to the gas absorption coefficient.

The residual for gas absorptance is defined as

$$R_\alpha = (^c \alpha_L - ^m \alpha_L)/^m \alpha_L = (^m \tau_L - ^c \tau_L)/(1 - ^m \tau_L) \quad (7)$$

The solution. - The solution is reached by reducing the residuals to an acceptably small value by appropriately changing the two variable parameters in the equation for the temperature profile and the one variable parameter in the equation for the pressure profile. This is done iteratively using the Newton-Raphson method (ref. 8, p. 175) because the equations are nonlinear. For two wavelengths of measurement each

iterative step involves the solution of the following three simultaneous equations for the increments  $\Delta y_j$  to the current value of the three variable parameters represented by  $y_j$ ,

$$\left. \begin{aligned} (1) \sum_j \left( \frac{1}{m_{N_{\lambda_1, L}}} \cdot \frac{\partial^c N_{\lambda_1, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_1, N} \\ (2) \sum_j \left( \frac{1}{m_{N_{\lambda_2, L}}} \cdot \frac{\partial^c N_{\lambda_2, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_2, N} \\ (3) \sum_j \left( \frac{1}{m_{\alpha_{\lambda_1, L}}} \cdot \frac{\partial^c \alpha_{\lambda_1, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_1, \alpha} \end{aligned} \right\} \quad (8)$$

Note that only one wavelength is needed for  $R_{\lambda_1, \alpha}$  to determine one pressure parameter. The derivatives in equation (8) are obtained numerically. The final value of the residuals is zero.

There are cases where there are more measurements than there are variable parameters. For these cases, where the final values of the residuals are not necessarily zero, a damped least-squares modification of equation (8) is used to find a solution at which

$$R_{\lambda_1, \alpha}^2 + \sum_i R_{\lambda_i, N}^2 \equiv R^2 = \text{a minimum} \quad (9)$$

where there are as many residuals  $R_N$  as there are  $i$  wavelengths, and there is only one residual  $R_\alpha$ . The damped least squares method is used in this program. Its derivation is in the second part of appendix B.

In addition to the solution for the profile parameters, an estimate is made of the error in the parameters that would be caused by stated random errors of radiometric measurements and tabulated absorption coefficients. (Typical orders of magnitude for these errors are 1 percent in radiation and 5 percent in absorption coefficient.) The error equation is derived in appendix B.

### Measurement of Gas Radiance and Transmittance

The actual gas radiance  $N_L$  and transmittance  $\tau_L$  are derived from measurements of detector (radiometer) output voltage  $V$  that is assumed to be proportional to incoming radiant power. The factor of proportionality (calibration factor) of the detector includes the effect of all optics between the radiometer element and the gas, but it need not be known explicitly if it remains constant for all measurements. The optics include, in addition to windows, lenses, and stops, a monochromator of bandwidth  $\Delta\lambda$  centered on wavelength  $\lambda$ . The following measurements of detector output voltage  $V$  are made:

- (a)  $V_0$ , where a calibrated source of radiance  $N_0$  is placed at the gas location, in place of the gas.
- (b)  $V_1$ , due to radiation from the gas.
- (c)  $V_2$ , where a stable comparison source radiates through the gas path, but the gas is absent.
- (d)  $V_3$ , when the comparison source radiates through the gas path in the presence of the gas.

By chopping the radiation from the comparison source at a unique, distinctive frequency, voltages  $V_1$  and  $V_3$  are distinguished from each other, and voltage  $V_3$  does not include gas radiation (ref. 1, p. 28).

These four measurements yield

$$N_L = N_0 \frac{V_1}{V_0}; \quad \tau_L = \frac{V_3}{V_2} \quad (10)$$

### Computation of Gas Radiance and Transmittance

The gas radiance, integrated over a narrow wavelength band  $\Delta\lambda$  centered at  $\lambda$  and over a path length  $L$ , is

$$N_L = \int_0^L N_\lambda^* \left( \frac{d\tau}{dx} \right) dx \quad (11)$$

where  $N_\lambda^*$  is the Planck radiation function

$$N_\lambda^* = \frac{c_1}{\lambda^5} (e^{c_2/\lambda T} - 1)^{-1}$$

and  $\tau$  is the gas transmittance over the path from 0 to  $x$ . The detailed justification for equation (11) is presented in reference 5.

The gas transmittance for a band  $\Delta\lambda$  is described by a band-model formulation for a nonisothermal gas based on equation (5) of reference 9. This formulation has been justified and applied in reference 2, and summarized in reference 10. For profiles with a large variation in temperature, the formulation as modified in references 3 and 11 is adopted. Other band-models can be found in the literature (ref. 12).

The transmittance  $\tau$  for a single gas is a function of the dimensionless optical depth  $u$  and is given by

$$\tau = \exp \left\{ \frac{-u\beta_e}{\left[ 1 + \left( \frac{\pi u}{2} \right) \right]^{1/2}} \right\} \quad (12)$$

For a mixture of  $q$  absorbing gases the combined transmittance is the product

$$\tau = \prod_{l=1}^q \tau_l \quad (13)$$

The optical depth of a path length  $x$  is

$$u = \frac{1}{\beta_e} \int_0^x k \left( \frac{\beta}{\beta_e} \right)^\eta dx \quad (14)$$

where  $k$  is the absorption coefficient at local temperature  $T$  and partial pressure  $p$  of the absorbing gas and  $\eta$  is an interpolation parameter. The parameter  $\beta$  is the local value of the line overlap parameter and is given by  $\beta = 2\pi\gamma/d$  where  $\gamma$  is the average line width, and  $d$  is the average line spacing. The definitions of  $u$  and  $\tau$  given here differ slightly in form from those of references 3 and 11 for reasons of computational expediency.

A modification in references 3 and 11 replaces the constant average  $\beta_e$  of reference 2 ( $\beta_{av}$  of ref. 4) by a cumulative average produced by weighting  $\beta(x)$  with the absorption coefficient, so that

$$\beta_e(x) = \frac{\int_0^x k \beta dx}{\int_0^x k dx} \quad (15)$$

The interpolation parameter  $\eta$  is given by one of two formulas

$$\left. \begin{aligned} \eta &= \frac{u + A_1}{u + A_2} & u > A_5 \\ \eta &= \frac{uA_3}{A_5 + uA_4} & u \leq A_5 \end{aligned} \right\} \quad (16)$$

where

$$A_5 = 1 + 0.185 (\beta/\beta_e) \quad (17)$$

Values for  $A_1$ ,  $A_2$ ,  $A_3$ ,  $A_4$ , and  $A_5$  are listed in table I in terms of  $(\beta/\beta_e)$ .

The computation for the initially assumed profiles  $T(x)$  and  $p(x)$  first determines all values of  $k$ ,  $\beta$ , and  $\beta_e$ , as functions of  $x$  from the band model data and equation (15). For example, tabulations of  $k_s$  and  $(\gamma/d)_s$  for  $H_2O$ ,  $CO_2$ , and  $CO$  may be obtained from reference 13 or, for  $H_2O$ , from references 14 and 15. (The subscript  $s$  here denotes the value at standard temperature and pressure.) Values of  $k_s$  in the tables are denormalized to the local gas temperature and partial pressure by

$$k = k_s p \frac{273}{T} \quad (18)$$

where  $p$  is in atmospheres and  $T$  is in kelvin. Similarly, the tabulated values of  $(\gamma/d)_s = \beta_s/(2\pi)$  may be used to obtain the local value as it is affected by the line-broadening effect of all gas components in accordance with the formula

$$\beta = \beta_s \left( \sum_k \alpha_k^* p_k + \sum_j \alpha_j^* p_j \right) \quad (19)$$

where  $p_j$ ,  $p_k$  are the partial pressures, and  $\alpha_j^*$ ,  $\alpha_k^*$  are the broadening coefficients for the  $k$  absorbing gases and  $j$  nonabsorbing gases. For the absorbing gas, values of  $\alpha^*$  are given in reference 16 and are listed in table II.

The path length  $0 \leq x \leq L$  is divided into increments  $\Delta x_i = x_i - x_{i-1}$  ( $i = 2, \dots$ ) and the values of  $k$ ,  $\beta/\beta_e$ ,  $\beta_e$  are determined at each station. Then, starting with the values  $\eta_1 = 0$ ,  $u_1 = 0$ , and  $\tau_1 = 1$  at  $x = 0$ , the following sequence of computations is made for each successive increment of path:

(1) Find  $u_i = u_{i-1} + \Delta u_i$  with equation (14), using  $k_i$ ,  $(\beta/\beta_e)_i$ ,  $(\beta_e)_i$ , and  $\eta_{i-1}$ .



(2) Find  $\eta_i$  with equations (10) and (11), using  $u_i$ . Linear interpolation in table I is used to find  $A_1$  to  $A_4$ , since the computation is relatively insensitive to these quantities. Equation (11) is used to find  $A_5$ .

(3) Find  $\tau_i$  with equation (12) using  $u_i$  and  $(\beta_e)_i$ .

For the numerical computation, equations (14) and (15) are written

$$u_i = \frac{1}{(\beta_e)_i} \sum_{l=2}^i k_l \left( \frac{\beta}{\beta_e} \right)_l^{\eta_{l-1}} \Delta x_l \quad (14a)$$

$$(\beta_e)_i = \frac{\sum_{l=2}^i k_l \left( \frac{\beta}{\beta_e} \right)_l^{\eta_{l-1}} \Delta x_l}{\sum_{l=2}^i k_l \Delta x_l} \quad (15a)$$

### Accuracy of the Solution

There are several sources of error that affect the accuracy of the solution. First there is the basic limitation of the functional forms assumed for the temperature and pressure profiles. Obviously not all situations encountered in practice can be accommodated by these functions with acceptable accuracy. For those cases other functional forms must be used. This basic limitation is demonstrated in the section "Application of the Program to an Experiment" where an example is worked out for a temperature profile that cannot be matched exactly by the assumed functional form for the temperature.

Another source of error is generated by the nature of the set of iteration equations for the parameters, equation (8). On the left side,

the matrix of derivatives may be poorly conditioned. The conditioning of the matrix is affected by the selection of the wavelengths of measurement. Proper selection of the wavelengths is treated in the next section.

The residuals on the right side of equation (8) are not exact quantities due to errors in their components  $c_{N_L}$ ,  $c_{\tau_L}$ ,  $m_{N_L}$ , and  $m_{\tau_L}$ . The measured quantities  $m_{N_L}$  and  $m_{\tau_L}$  contain an experimental random measurement error and the computed quantities  $c_{N_L}$  and  $c_{\tau_L}$  are in error because of uncertainties in the tabulated gas parameters  $\beta_s$  and  $k_s$ . There are also errors due to deficiencies in the band model used in the gas transmittance calculation. These deficiencies in the model are covered in the references cited in the previous section and will not be covered further here. Thus, even if the computer program succeeds in finding a solution that reduces the residual values to zero, the computed parameters are still in error due to the residual errors. By using equations (6) and (7) it can easily be shown that the residual errors at the solution,  $\delta R_N$  and  $\delta R_\alpha$  are given by

$$\delta R_N = \frac{\delta c_{N_L}}{c_{N_L}} - \frac{\delta m_{N_L}}{m_{N_L}} \quad (20a)$$

$$\delta R_\alpha = \frac{m_{\tau_L}}{1 - m_{\tau_L}} \left( \frac{\delta m_{\tau_L}}{m_{\tau_L}} - \frac{\delta c_{\tau_L}}{c_{\tau_L}} \right) \quad (20b)$$

where  $\delta c_{N_L}$ ,  $\delta m_{N_L}$ ,  $\delta c_{\tau_L}$ , and  $\delta m_{\tau_L}$  are the errors in  $c_{N_L}$ ,  $m_{N_L}$ ,  $c_{\tau_L}$ , and  $m_{\tau_L}$ , respectively.

To proceed further it is necessary to specify the errors in the measured and computed quantities. It will be assumed that all measurements have the same probable error given by  $|\delta^m V / m_V|$  and that the computed values for  $N_L$  and  $\tau_L$  have random errors due to the uncertainty  $|\delta k_s / k_s|$  in published  $k_s$  values.

The uncertainty in the value of  $\beta_s$  will be neglected. Thus, only two random errors will be considered,  $|\delta^{m_V}/m_V|$  and  $|\delta k_s/k_s|$ .

Using equations (10) and the definition  $m_{\alpha_L} = 1 - m_{\tau_L}$  it can be easily shown that

$$\left(\frac{\delta^{m_{N_L}}}{m_{N_L}}\right)^2 = \left(\frac{\delta^{m_V}}{m_V}\right)^2 \quad (21a)$$

$$\left(\frac{\delta^{m_{\tau_L}}}{m_{\tau_L}}\right)^2 = 2 \left(\frac{\delta^{m_V}}{m_V}\right)^2 \quad (21b)$$

$$\left(\frac{\delta^{m_{\alpha_L}}}{m_{\alpha_L}}\right)^2 = 2 \left(\frac{\tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta^{m_V}}{m_V}\right)^2 \quad (21c)$$

To estimate the random errors in the computed quantities, assume a simplified transmittance equation given by  $c_{\tau_L} = \exp(-k p L)$ . It can then be shown that

$$\left(\frac{\delta^{c_{N_L}}}{c_{N_L}}\right)^2 = \left(\frac{\delta^{c_{\alpha_L}}}{c_{\alpha_L}}\right)^2 = \left(\frac{\tau_L \ln \tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta k}{k}\right)^2 \quad (21d)$$

The above quantities when substituted into equations (20a) and (20b) give for the squares of the random residual errors

$$\delta R_N^2 = \left(\frac{\delta^{m_V}}{m_V}\right)^2 + \left(\frac{\tau_L \ln \tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta k}{k}\right)^2 \quad (22a)$$

$$\delta R_{\alpha}^2 = \left( \frac{\tau_L}{1 - \tau_L} \right)^2 \left[ 2 \left( \frac{\delta^m_V}{m_V} \right)^2 + (\ln \tau_L)^2 \left( \frac{\delta k}{k} \right)^2 \right] \quad (22b)$$

The random residual error  $\delta R_N^2$  (eq. (22a)) depends on the error  $\delta k/k$ . An alternative form that eliminates this dependence is to substitute for equation (6) the expression

$$\bar{R}_N = (c\bar{N}_L - m\bar{N}_L)/m\bar{N}_L \quad (23)$$

where  $\bar{N}_L$  is an apparent radiance defined by

$$\bar{N}_L = N_L / \alpha_L \quad (24)$$

By repeating the previous procedure it can be shown that

$$\delta \bar{R}_N^2 = \left[ 1 + 2 \left( \frac{\tau_L}{1 - \tau_L} \right)^2 \right] \left( \frac{\delta^m_V}{m_V} \right)^2 \quad (25)$$

The quantity  $\delta \bar{R}_N^2$  is less than  $\delta R_N^2$  whenever

$$(\ln \tau_L)^2 > \frac{2(\delta^m_V/m_V)^2}{(\delta k/k)^2} \quad (26)$$

Because experience has shown that  $\delta \bar{R}_N^2$  is less than  $\delta R_N^2$  in most practical situations, the computer program presented herein uses  $\bar{R}_N$  given by equation (23) instead of  $R_N$  given by equation (6) for the residuals in equations (8) or (9).

Equations (25) and (22b) give a measure of the uncertainties in the zero values for the residuals at the solution. These expressions are used in the computer program following the procedure outlined in appendix B to compute the random errors in the temperature and pressure profile parameters.

## Selection of Wavelengths of Measurement

The wavelengths differ principally in their associated gas absorption coefficients. Figure 2 shows the absorption coefficient  $k$  for the  $2.7 \mu\text{m}$  band of  $\text{H}_2\text{O}$ . At wavenumbers near the center of the band ( $3704 \text{ cm}^{-1}$ ),  $k$  decreases with temperature; at the wings,  $k$  increases with temperature. Substantial differences in  $k$  exist, especially at a low temperature. Another difference due to wavelength is caused by a greater increase of the Planck-function radiance with temperature at the shorter wavelengths. Since the variation of  $k$  with wavelength is the phenomenon that enables the profile to be determined, large differences would be expected to be favorable.

The wavelengths are selected to maximize accuracy of the solution, and equally important, to avoid an incorrect second solution that can exist. This preliminary selection is performed through an auxiliary computer program WAVES. The selection procedure will be illustrated with both modes of the temperature profile function, equations (1) and (2).

Avoiding an incorrect solution. - The WAVES program uses the following procedure: For assumed values of the two variable temperature parameters in equations (1) or (2), as applicable, and one variable pressure parameter in equation (3), the quantities  $c_{\bar{N}_L}$  and  $c_{\tau_L}$  are computed for each wavelength. These computed quantities are substituted for presumed error-free measurements  ${}^m\bar{N}_L$  and  ${}^m\tau_L$  of the assumed profiles. Then, taking one wavelength at a time, one parameter  $w$  of the temperature profile is assigned a value different from that assumed. The quantities  $c_{\bar{N}_L}$  and  $c_{\tau_L}$  change. Then, new values of the other temperature parameter and the pressure parameter are found by iteration that restore the equalities  $c_{\bar{N}_L} = {}^m\bar{N}_L$  and  $c_{\tau_L} = {}^m\tau_L$ . This procedure is repeated for a number of assigned values of the temperature profile parameter  $w$ , and the results are tabulated by the program.

For each wavelength, the tabulation can be plotted as a curve with the independently varied parameter  $w$  as abscissa and the dependent temperature parameter as ordinate. The intersection of any two curves is a two-wavelength solution for a temperature profile.

As an example, assume a path length of 100 cm, hydrogen-air combustion at 1 atm total pressure having  $H_2O$  pressure parameters  $p_c = 0.35$  atm,  $p_w = 0.30$  atm, and  $n_p = 0.5$ . Computations are made for wavelengths in the  $2.7 \mu m$  band of  $H_2O$ . Results are plotted in figure 3 for the profile of figure 1(a) with  $n_T$  as the independent parameter and  $T_c$  as dependent, and in figure 4 for the profile of figure 1(b) with  $T_w^*$  as the independent parameter and  $T_c$  as dependent, with no wall boundary layer ( $x_1 = 0$ ). To facilitate plotting and to emphasize differences in the curves, the ordinate  $Y$  of the graph is tabulated by the program as a function

$$Y = Z + \xi(w - w_o) \quad (27)$$

where  $Z$  is the dependent parameter,  $w$  is the independent parameter,  $w_o$  is the originally-assumed value, and  $\xi$  is chosen by the program as described in appendix C. All curves intersect at the true solution. Some pairs of curves intersect at a second point that is an incorrect solution. For example, in figure 4, wavenumbers  $3500$  and  $3100 \text{ cm}^{-1}$  intersect at approximately  $T_w^* = 2200 \text{ K}$  and  $T_c = 1840 \text{ K}$ . A solution by the computer program converged to  $T_w^* = 2223 \text{ K}$  and  $T_c = 1873 \text{ K}$  from a starting point  $T_w^* = 2300 \text{ K}$  and  $T_c = 1800 \text{ K}$ . To assure convergence to the true solution, a pair of curves should have increasing separation with distance from the true solution. Accuracy is greatest when there is a large difference of slope between a pair of curves. Where two curves become parallel, accuracy approaches zero.

Inspection of figures 3 and 4 show that no single pair of wavelengths is satisfactory for all profiles. Acceptable pairs of wavenumbers in figure 3 are  $(3100, 3550 \text{ cm}^{-1})$  and  $(3100, 3775 \text{ cm}^{-1})$ . The  $2000 \text{ K}$  almost-isothermal profile that led to figure 4 shows an acceptable pair

(3500, 3100  $\text{cm}^{-1}$ ) for  $T_w^*$  below 2000 K, and an acceptable pair (4100, 3400  $\text{cm}^{-1}$ ) for  $T_w^*$  above 2000 K.

Tests of the pressure profile when the two pressure parameters  $p_w$  and  $p_c$  were assumed to be variables, and only  $T_c$  was variable, gave curves nearly alike for all wavelengths. Thus, poor accuracy of the computed pressure profile makes this technique unacceptable; it is therefore necessary to limit oneself to only one variable pressure parameter. The reasons for this poor accuracy are (1) that radiance and absorption coefficient usually vary more strongly with temperature than they do with pressure and (2) that the measurement of  $\tau_L$ , equation (10) which is the principal source of information about the pressure, is sensitive only to the integral of pressure over the path and not to local values of pressure, whereas  $N_L$  (which is the principal source of information about temperature) is sensitive to local temperature.

Maximizing accuracy of the solution. - The program that led to figures 3 and 4 does not provide an estimate of the error for pairs of wavelengths. This estimate is provided by the main program PROFIL (MODE=1). The error estimate is made by pairing one principal wavelength with each of all the other wavelengths to be tested. For each dependent profile parameter, the program tabulates the error in the parameter due to assigned errors of the radiation-measurement voltages  $V$  and the tabulated absorption coefficient  $k_s$ .

As an example, such tabulated values are plotted in figure 5 for the parameter  $T_c$  with the profiles and some of the wavelengths of figure 3. The assumed errors were 1 percent in  $V$  and 5 percent in  $k_s$ . Another example with the same assumed error is plotted in figure 6 for  $T_c$  with the profiles and some of the wavelengths of figure 4. These errors are for profiles with  $T_c = 2000$  K, and the range of values covered by the abscissa parameter. The errors are consistent with the slope-difference of curve pairs in figures 3 and 4. The error is minimized in figure 6 with wavenumber pairs (4100, 3400  $\text{cm}^{-1}$ ) above 1950 K, and (3500, 3100  $\text{cm}^{-1}$ ) below 1850 K.

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All four of these wavenumbers have been used simultaneously in a least squares solution by the program PROFIL (MODE=3). The resulting error also plotted in figure 6(b), shows improvement at all values of  $T_w^*$ . The effect of path length on the error at  $T_w^* = 1200$  and  $2000$  K is listed in table III, for this four-wavelength combination. The error varies approximately as the inverse square root of the path length, in this example.

### PROGRAM DESCRIPTION

The accuracy of the temperature profile found with measured data is dependent on the pressure and temperature profiles, path length, and wavelengths selected for measurement. It is desirable as a preliminary step to assume realistic values for the path length and pressure and temperature profiles for the absorbing gas, and then to select wavelengths and estimate the accuracy of the temperature profile parameters as was illustrated in the Selection of Wavelengths of Measurement section.

A separate main program WAVES (described in "Avoiding an incorrect solution") is designed for the selection of wavelengths. Using these wavelengths, a principal main program PROFIL gives results in three modes of operation:

**MODE=1:** This program computes the error in the dependent profile parameters that would be caused by assigned random errors of radiometric measurements and tabulated absorption coefficients. For given values of all profile parameters, gas radiance and transmittance are calculated and the parameter errors are computed as in appendix B. Actual radiometric measurements are not required. The estimate may be made for any pair of wavelengths consisting of one "principal" wavelength and any one of up to seven others.

**MODE=2:** This program computes values for the dependent profile parameters using the iterative procedure described previously. Limits are assigned to the dependent parameters by the user; if a limit is



reached during the iteration, that parameter becomes fixed, and the iteration proceeds for the remaining dependent parameters. When a least-squares solution is used, the magnitude of the final root-mean-square residual  $R$  (eq. (9)) is also provided. In addition, using the same procedure as in  $\text{MODE}=1$ , the error in the dependent parameters that would be caused by assigned random errors in the radiometric measurements and tabulated absorption coefficients is computed.

$\text{MODE}=3$ : This program is used to find the change of temperature profile that would be caused by a change in one of the independent profile parameters. A second set of data cards is required that incorporate the change. Starting with an assumed profile and gas-property data, the resulting radiance and transmittance that would be measured are calculated. The second set of data cards is then introduced to change one of the independent profile parameters, and the computation in  $\text{MODE}=2$  is performed using the previous radiance and transmittance values to yield a revised profile. This process is useful in identifying independent profile parameters to which the temperature profile is unusually sensitive.

The flowchart for program PROFIL is figure 7. After reading input data and calculating some initial conditions, the main program calls subroutines TEMP that calculates profiles, and TRANS that calculates gas transmittance and radiated flux. The subroutines are principally a computation using equations presented in the text. The equation numbers appear on comment cards in the listings.

The test result  $\text{DONE}=1$  is obtained when (1) the number of iterations reaches a preset number, or (2) when the root-mean-square sum of all residuals is less than  $10^{-4}$ , or (3) when the fractional change of the variable parameters per iterative step has become less than  $10^{-4}$  for  $T_w$  and  $T_c$ , and less than  $10^{-3}$  for  $p_c$  and  $n_T$ . Criterion (3) is needed when there are more residuals than variable parameters, because the residuals then reach a nonzero minimum.

A subsidiary loop of moderate complexity determines the variable parameter increments and tests the parameters for exceeding their

limits. The loop contains a control index number **KEY** that manipulates the index of FORTRAN DO statements as follows. The variable profile parameters in equation (1) are  $n_T$ ,  $T_c$ ,  $p_c$ ,  $T_w^*$ . They are represented by a FORTRAN subscripted variable **PA(K)** that is controlled by a DO index  $K=K1, K2, K3$ . An index initially  $K=1, 3, 1$  selects parameters  $n_T$ ,  $T_c$ ,  $p_c$  for the profiles of figure 1(a) and  $K=2, 4, 1$  selects parameters  $T_c$ ,  $p_c$ ,  $T_w^*$  for the profiles of figure 1(b).

Any parameter in either profile can be fixed when it reaches an assigned limit by changing the index parameters  $K1, K2, K3$ . This is done by setting  $K1, K2, K3$  equal to the subscripted quantities **KEY1(KEY)**, **KEY2(KEY)**, **KEY3(KEY)** that can be manipulated. The subscript **KEY** can select any combination of numbers for  $K1, K2, K3$  as shown in table IV. The variable parameters for each **KEY** are also listed. By designating the profiles of figure 1(a) as **PROF=1** and the profiles of figure 1(b) as **PROF=2** the table is valid for **PROF=1** and **PROF=2** when subsequent additions are made,  $K1=K1-1+PROF$ , and  $K2=K2-1+PROF$ . The initial profile with no limits reached is **KEY=1**.

Before entering the loop, **KEY=1**, and  $K1, K2, K3$ , are set as in the table. This frees the currently fixed parameters to return inside their limits during every iterative step. Thus, on first entering the loop, all three parameters (corresponding to **KEY=1**) are incremented and compared with their limits. If the  $K'$ th parameter is within its limit, a limit-indicating variable **LIM (K4)=0** where  $K4=K-PROF+1$  (to be valid for **PROF=1** and **PROF=2**). If the  $K'$ th parameter is outside the limit, **LIM(K4)=1**. The value of **KEY** is a number from 1 to 8 given by

$$KEY=1+4* LIM(1)+2* LIM(2)+LIM(3)$$

If this new value of **KEY** is not 1 or 8 the preceding procedure of this paragraph is repeated only once from the start of the loop with the new value of **KEY**, and the corresponding  $K1, K2, K3$  to find new parameter increments and tentative new parameter values. The loop is then exited, the tentative new parameter values are then accepted,

and the iteration proceeds. At the solution the error of the profile parameters is estimated. The program listing with a FORTRAN symbol list is appendix D. The subroutine listings are appendixes E and F.

The flow chart for program WAVES is figure 8. After reading the input data, the program (following the procedure described in Selection of Wavelengths of Measurement) first sets  ${}^mN_L = {}^cN_L$  and  ${}^m\tau_L = {}^c\tau_L$  for the initial profile. Then follow three nested loops. An outer DO loop for selecting each given wavelength, a DO loop for assigning given values to one independent variable profile parameter; and an iteration loop like PROFIL that finds the other two dependent variable parameters. If a variable parameter reaches a limit during iteration, the iteration is ended. After completion of the two DO loops the results are tabulated. The program listing, with FORTRAN symbols not used in program PROFIL, is appendix G.

Successive problems in the same run may omit input data that is not changed. (Both PROFIL and WAVES programs.) The READ data is omitted by not putting IREAD=1 in the NAMELIST data. In the NAMELIST, the data-input parameters of temperature,  $T_w$ ,  $T_c$ , and  $n_T$ , and pressure,  $p_w$ ,  $p_c$ , and  $n_p$  are given starting values that are not changed by the program because they are replaced by different internal symbols for computation. After computation the values of the internal symbols are printed, but with the corresponding symbols of the initial data-input parameters.

## PROFIL PROGRAM USE

### Input

The input consists of four types of data: (1) computer program control constants (2) measurements of gas radiance and transmittance at selected wavelengths (3) tabulations from the literature of gas transmission parameters at selected wavelengths and (4) independently determined or estimated profiles of partial pressures of the gas reaction products.

The collected input data are read in with a FORTRAN NAMELIST for single-subscript quantities, followed by a FORTRAN READ STATEMENT for multiple-subscript quantities. An example in appendix H shows this input data in the same format as punched on cards, for MODE=1, five wavenumbers, and two gases,  $H_2O$  and  $N_2$ . The data conform to the following specifications.

NAMELIST DATA. - The following list gives the FORTRAN symbol with its subscripted maximum dimension and equivalent algebraic symbol, in the NAMELIST sequence.

<u>FORTRAN symbol</u>	<u>Algebraic symbol</u>	<u>Description</u>
MODE		<p>MODE=1 finds error estimate of pairs of wavenumbers consisting of the first wavenumber paired with each succeeding wavenumber</p> <p>MODE=2 finds solution to given measurements, with error estimate</p> <p>MODE=3 finds gas radiance and transmittance for given input, then requires NAMELIST repeated that may have changes from the first NAMELIST, and finds solution the same as MODE=2</p>
PROF		<p>PROF=1 profile figure 1(a), variable parameters TC, PC, NT. PROF=2 profile figure 1(b), variable parameters TW, TC, PC, with given boundary layer wall temperature TWB, thickness X(JB)</p>

<u>FORTTRAN symbol</u>	<u>Algebraic symbol</u>	<u>Description</u>
IREAD		IREAD=1 requires READ data for GAS, ALPH, KTAB, BTAB. With IREAD=1 omitted, READ data must be omitted
PATH	L	Test section path length, cm
I1 (8 maximum)		Number of wavenumbers for com- putation (when IREAD=1, I1 must equal number of data cards for KTAB and BTAB)
WAVE(8)	$\lambda$	Wavenumber $\text{cm}^{-1}$
MRL(8)	$m_{N_L}$	Measured radiance $W, \text{cm}^{-1}$ $\text{cm}^{-2} \text{ster}^{-1}$ (eq. (10))
MTAUL(8)	$m_{\tau_L}$	Measured transmittance (eq. (10))
ERRV		Percent error of radiation meas- urement
ERRK		Percent error of tabulated ab- sorption coefficient
TW	$T_w, T_w^*$	Gas temperature, K, at wall. For PROF=2 with boundary layer, $T_w^*$ approximates free stream temperature near the wall
TC	$T_c$	Gas temperature, K, on axis
NT	$n_T$	Gas temperature profile equation exponent
TWB	$T_w$	Gas temperature, K, at wall for PROF=2 with boundary layer

<u>FORTTRAN symbol</u>	<u>Algebraic symbol</u>	<u>Description</u>
JB (minimum is 1 at wall)		Index for X(JB) giving distance x from wall where boundary layer ends, for PROF=2
UPLIM(4)		Upper limit of profile parameters TW, TC, PC, NT
BOTLIM(4)		Lower limit of profile parameters TW, TC, PC, NT
L1 (3 maximum)		Number of absorbing gases
L2 (6 maximum)		Number of absorbing plus non-absorbing gases
PS	$p_s$	Gas static pressure, constant along optical path
PC(6)	$p_c$	Partial pressure of each gas, on axis
NP(6)	$n_p$	Pressure profile equation exponent of each gas
PW(6)	$p_w$	Partial pressure of each gas, at wall
NK (8 maximum)		Number of tabulated values of KTAB read in for data
TKTAB(8)		Temperatures at which values of KTAB are tabulated in READ data
NB (8) maximum)		Number of tabulated values of BTAB read in for data
TBTAB(8)		Temperatures at which values of BTAB are tabulated in READ data

<u>FORTTRAN symbol</u>	<u>Algebraic symbol</u>	<u>Description</u>
J1 (41 maximum)		Number of stations along optical path. Must be odd. Omit if J1=21 in DATA-statement of program is acceptable.
Z(J)		Station distance ratio, from wall to center, as fractional value 0 to 1. Omit if list in DATA-statement of program is acceptable. Maximum $J=(J1+1)/2$
ITER		Maximum number of iterations

READ statement data. - The following list gives the FORTRAN symbol with its subscripted maximum dimension, the format of each card, and the equivalent algebraic symbol.

<u>FORTTRAN symbol</u>	<u>Format</u>	<u>Algebraic symbol</u>	<u>Description</u>
GAS(6)	6A6		Names of all gases
ALPH(3, 6)	(12F6.0)	$\alpha^*$	Broadening factor for up to 3 absorbing gases by up to 6 total number of gases. Card sequence is one card for each L1 absorbing gases. Each card lists the broadening factor for each of L2 gases.

<u>FORTTRAN</u> <u>symbol</u>	<u>Format</u>	<u>Algebraic</u> <u>symbol</u>	<u>Description</u>
KTAB(8, 3, 8)	(12F6.0)	$k_o$	Absorption coefficient at S. T. P. for up to I1=8 wavenumbers, L1=3 gases, NK=8 tabulated points. Card sequence is one set of cards for each of L1 absorbing gases. Each set has I1 cards corresponding to the wavenumbers in NAMELIST. Each card lists absorption coefficients corresponding to temperatures TKTAB in NAMELIST.
BTAB(8, 3, 8)	(12F6.0)	$\beta_o$	Line-broadening coefficient at S. T. P. for up to I1=8 wavenumbers, L1=3 gases, NB=8 tabulated points. Card sequence same as for KTAB above. Each card lists broadening coefficients corresponding to temperature TBTAB in NAMELIST.

The two gas transmittance parameters KTAB and BTAB depend on temperature. For H<sub>2</sub>O and CO<sub>2</sub>, they are tabulated in references 10 to 12 with KTAB and BTAB normalized to S. T. P. The program interpolates between tabulated values to find a tabulated value at local temperature, then denormalizes to obtain KK and BB at local temperature and pressure in accordance with equations (18) and (19). Linear interpolation is used. If the profile temperature is outside the temperature range of the tabulation, KK and BB are limited to the extreme tabulated value. It is thus desirable to prepare the tabulation with a temperature range running from the lower to upper limits appearing on other input cards for the profile temperatures TC, TW, and TWB.



## Output

An example of the output shown in appendix H for **MODE=1** and **PROF=2** consists of four parts:

1. The input **NAMelist** and **READ** data.
2. Estimated error of the profile parameters caused by the residuals, equations (20) and (25), due to the errors of measurement **ERRV** and of absorption coefficient **ERRK**. The example has **ERRV=1** percent and **ERRK=5** percent. The example shows four wavenumbers 3100, 3400, 4100, and 3000  $\text{cm}^{-1}$  successively paired with the first wavenumber 3500  $\text{cm}^{-1}$ . The first pair have residuals  $\bar{R}_N = 2.0$  and 3.2 percent at 3500 and 3100  $\text{cm}^{-1}$ , and  $R_\alpha = 4.4$  percent at 3500  $\text{cm}^{-1}$ . These residuals cause the listed three errors for each parameter, and their rms total.
3. Transmittance at each wavenumber.
4. Temperature and pressure profiles.

An example shown in appendix I for **MODE=3** was in the same run and followed the preceding example. The **READ** statement data and most items in the **NAMelist** were not changed. Thus, only two data cards were required. The first four wavenumbers were used in a least squares solution. Appendix I shows the input data in the same format as punched on cards. The first **NAMelist** has **MODE=3** and **I1=4**. The required second **NAMelist** has a change in the nonvariable pressure parameter,  $p_w = 0.36$  replacing  $p_w = 0.30$ . The output consists of four parts:

1. The first input **NAMelist** and the second **NAMelist** that differs by the new  $p_w = 0.36$  and an internal change to **MODE=2**. Because **IREAD=1** was omitted, the **READ** data were not required or printed out.
2. Each iteration step lists the parameters, the residuals  $\bar{R}_N$  for each wavenumber, the residual  $R_\alpha$  for the first wavenumber, the rms total residual, and a step size that is the total fractional change of the variable parameters. In this example the 20 percent change of  $p_w$  from 0.30 to 0.36 caused errors  $\delta T_c = 1.2$  K or 0.06 percent,  $\delta p_c = -0.019$  atm or 5.4 percent, and  $\delta T_w = 14$  K or 0.5 percent. Because

four wavenumbers were used (I1=4) the iteration was terminated by the small step size, as the residuals became stationary and remained nonzero.

3. Estimated error of the profile parameters caused by the residuals  $\delta R_N$  and  $\delta R_\alpha$ . The percent errors are  $\delta T_c = 3.5$  percent,  $\delta p_c = 7.1$  percent and  $\delta T_w = 6.6$  percent. These errors are much larger than those listed in (2) above caused by the change of  $p_w$ .

4. Temperature and pressure profiles.

The output in MODE=2 is the same as MODE=3 without the first NAMELIST.

## WAVES PROGRAM USE

### Input

The input includes all quantities listed for PROFIL. Three additional quantities in the NAMELIST select the independent temperature parameter and assign values to it that differ from the initial value. The independent parameter is determined by index K4 of PA(K4), where K4=1 for  $n_T$ , K4=2 for  $T_c$ , and K4=4 for  $T_w$ . The program selects the dependent parameter in accordance with the profile, either PROF=1 or PROF=2.

<u>FORTRAN symbol</u>	<u>Description</u>
K4	Index of independent variable temperature parameter PA(K4)
NPA	Number of values of PA1 to be used, up to ten.
PA1(10)	Values that may be assigned to PA(K4).

### Output

An example in appendix J shows the input data in the same format as punched on cards for four wavenumbers and two gases,  $H_2O$  and  $N_2$ . The output has four parts:

1. The NAMELIST and READ data
2. Temperature and pressure profiles
3. At each solution found by iteration, the four variable profile parameters, wavenumbers, number of iterations, final rms residual
4. Tabulations of dependent parameter against independent parameter for each solution in (2), with the dependent parameter modified for plotting by equation (27) with the constant  $\xi$

Examples of plotted tabulation are figures 3 and 4.

### DIAGNOSTICS

A warning is printed each time:

1. The pressure of all absorbing gases exceeds the static pressure at any point on the pressure profile.
2. During iteration when a variable parameter reaches the assigned upper or lower limit.

### APPLICATION OF THE PROGRAMS TO AN EXPERIMENT

Three steps are used to determine whether this method will be sufficiently accurate for an application. These steps will be summarized in this section, and an example of an application will be given. The steps are:

1. Estimates of the temperature and pressure profiles are made, and the profile equations are selected.
2. Some wavenumbers for measurement are selected, and then compared using graphs of the output of the WAVES program. This was demonstrated in figures 3 and 4.
3. Accuracy of the dependent profile parameters is determined for the best pairs of wavenumbers selected from graphs in step (2). This was demonstrated in figures 5 and 6. Tests with the PROFIL program in MODE=3 may be run with a perturbation of an independent profile parameter. The resulting change of all dependent profile parameters

may be judged acceptable or excessive. This is demonstrated in appendix I.

Based on the results of steps (2) and (3), it can then be determined if there exists a pair of wavenumbers that lead an acceptably low level of random error in the computed parameters. The experimental measurements are then made at the wavenumbers chosen and the results serve as inputs to the PROFIL program in MODE=2 for determining the temperature and pressure profiles.

An example of the PROFIL program is given to illustrate the limitation of the assumed functional form of the temperature profile as described by two variable parameters. An assumed profile with a high temperature core is shown in figure 9. This profile cannot be matched exactly by equations (1a) or (1b). The pressure profile is the same as used in other examples; hydrogen-air combustion at 1 atm, parameters  $p_w = 0.30$  atm,  $p_c = 0.35$  atm, and  $n_p = 0.50$ .

By following steps (1) to (3) given at the beginning of this section it was found that wavenumbers of  $3100\text{ cm}^{-1}$  and  $3500\text{ cm}^{-1}$  were suitable for use. The radiance and transmittance of the assumed profile were calculated at these wavenumbers to represent error-free measurements. With these measurements as input data, the PROFIL program in MODE=2 found the profiles with equations (1a) and (1b) that are plotted in figure 9. The profiles in figure 9(a) and (c) use an independently determined wall temperature  $T_w = 1100\text{ K}$  that was made 100 K lower than the assumed profile  $T_w = 1200\text{ K}$ . This represents an error of  $T_w$ . The difference between the assumed and computed profiles is an error of approximation due to limitations in the ability of the profile functions to assume an arbitrary shape. This may be compared with the error band that is due to an assumed radiance measurement error of one percent and a tabulated absorption coefficient error of five percent.

The PROFIL program data cards and output for figure 9(a) are shown in appendix K. The output format is the same as shown and described for MODE=3, appendix I, without the first namelist.

### CONCLUDING REMARKS

All of the examples presented in this report were for hydrogen-air combustion at a pressure of 1 atmosphere with a path length of 100 cm. These reactants produce  $\text{H}_2\text{O}$  as the absorbing gas. It was shown in table III that the random error in the computed profiles decreases with increasing path length. It can also be shown that the random error in the profiles will decrease with increasing pressure or by using a gas with greater absorptance such as  $\text{CO}_2$ . However, in applications where the path length, gas pressure, and gas type are all fixed, a user of this computer program has only the choice of the wavelengths of measurement at his disposal in order to attempt to bring the computed profile errors within acceptable bounds.

## APPENDIX A

## SYMBOLS

$A$	matrix of first derivatives
$A_1$ to $A_5$	coefficients in eqs. (16) and (17)
$a$	element of $A$
$B$	matrix of second derivatives
$b$	element of $B$
$d$	average spectral line spacing
$k$	gas absorption coefficient, $\text{cm}^{-1}$
$L$	total path length of profile
$n_T$	exponent in equation for temperature profile
$n_p$	exponent in equation for pressure profile
$N_L$	actual gas radiance
$m$	temperature-gradient, eq. (2)
$N^*$	radiance by Planck function
$\overline{N}_L$	apparent radiance defined by eq. (24)
$p$	partial pressure of absorbing gas
$p_S$	static pressure
$q$	number of absorbing gases
$R$	total residual, rms value; also column matrix of residuals
$R$ (subscripted)	residual, eq. (6) based on $N_L$ and $\tau_L$
$\delta R$ (subscripted)	residual errors, eqs. (20a) and (20b)
$\overline{R}$ (subscripted)	residual, eqs. (23), based on $\overline{N}_L$
$\delta \overline{R}$ (subscripted)	residual error, eq. (25)

$T$	temperature
$T_w^*$	temperature parameter in temperature profile, eq. (2), fig. 2(b)
$u$	dimensionless optical depth
$V$	detector output voltage
$w$	independently varied parameter
$x_1$	boundary layer thickness
$x$	distance along profile or optical path
$y$	dimensionless path-length ratio, eq. (1) or variable parameter, eq. (8), (B1)
$Y$	graph-plotting ordinate, eq. (27)
$Z$	dependent parameter
$z$	dimensionless path-length ratio, eq. (2)
$\alpha_L$	absorption factor of gas
$\alpha^*$	spectral line-broadening coefficient
$\beta$	spectral-line overlap factor, band model parameter
$\gamma$	average spectral line width
$\eta$	interpolation parameter
$\lambda$	wavelength
$\rho$	gas density
$\tau_L$	transmittance
$\zeta$	graph-plotting constant, eq. (27)

Subscripts:

$c$	centerline of profile
$s$	standard conditions
$w$	ends of profile (wall)

$p$	pressure
$T$	temperature
$N$	radiance
$e$	effective value
$L$	total path length
$\alpha$	absorptance
$\lambda$	wavelength
$o$	initial conditions

Superscripts:

$c$	computed
$m$	measured

Running indices:

$i$	path length; also wavelength in eq. (6)
$j$	absorbing gases
$k$	nonabsorbing gases; also dependent parameters in matrix solution
$l$	intermediate index for path length



## APPENDIX B

## PROFILE PARAMETER ERROR ESTIMATE

In order to use matrix notation and FORTRAN coding, the four variable parameter symbols  $T_c$ ,  $T_w$ ,  $p_c$ , and  $n_T$  are replaced by one subscripted symbol  $y_j$ . Only three of these are treated as dependent variables at any one time.

Due to random errors in the measured and computed terms that form the residuals  $R_N$  and  $R_\alpha$ , there will also be a random error  $\delta y_j$  associated with each parameter  $y_j$ . The random errors in the residuals are denoted by  $\delta R_i$  (see eqs. (20) and (22)).

When the number of equations is equal to the number  $m$  of unknowns, the errors  $\delta y_j/y_j$  are a solution of  $m$  equations in  $m$  unknowns,

$$\sum_{j=1}^m \frac{\partial R_i}{\partial (\delta y_j/y_j)} \cdot \left( \frac{\delta y_j}{y_j} \right) = \delta R_i \quad i = 1, m \quad (B1)$$

or, in matrix notation,

$$A \left( \frac{\delta y}{y} \right) = \delta R \quad (B2)$$

The elements of  $A$  are partial derivatives in equation (B1) that are found by numerical differentiation in the computer program.

When the number  $n$  of equations is greater than the number  $m$  of unknowns, the least squares method is applied to give the equation

$$A^T A \left( \frac{\delta y}{y} \right) = A^T \delta R \quad (B3)$$

where  $A^T$  is the transpose of  $A$ . This can be written as

$$\frac{\delta y}{y} = \left[ (A^T A)^{-1} A^T \right] \delta R \quad (B4)$$

which is equivalent to the set of  $n$  equations, and  $m$  unknowns,

$$\sum_{i=1}^n \frac{\partial(\delta y_j / y_j)}{\partial R_i} \cdot \delta R_i = \frac{\delta y_j}{y_j} \quad (B5)$$

Each term in equation (B5) isolates the contributions of  $\delta R_i$  to the total error of each variable parameter. Since the sign of  $\delta R_i$  is equally likely to be plus or minus, the rms total for all  $n$  terms gives the estimated error for each  $j$  parameter.

### Damped Least Squares Method

Where an iterative method of solution is used to deduce the profile parameters from experimental measurements, the profile parameter fractional increments are  $\delta y_j / y_j$  for an iterative step. The increment size is determined by the residuals  $R_i$  which are to be minimized. These residuals are:  $\bar{R}_N$ , equation (23), at each wavelength  $\lambda_i$ ;  $R_\alpha$ , equation (7), at wavelength  $\lambda_1$ . The least squares method, equation (B3), minimizes  $R$  by reducing  $A^T R$  to zero. Near the solution where  $-A^T R$  becomes zero, damping is required to prevent oscillation of the variable parameters about the solution (refs. 17 and 18). When a damping factor is selected in accordance with equation (11) of reference 19, equation (B3) becomes

$$\left[ A^T A + (p/q)Q \right] \frac{\delta y}{y} = -A^T R \quad (B6)$$

The elements of matrix  $A$  are first derivatives of the residual, given by

$$a_{ij} = y_j (\partial R_i / \partial y_j) \quad (B7)$$

where  $R_i$  is by definition a fractional value. The transpose of  $A$  is  $A^T$ . The damping increases the principal diagonal of  $A^T A$  by a factor  $1 + (p/q)$  where  $Q$  is a diagonal matrix whose elements are the principal-diagonal elements of  $A^T A$ . The number  $q$  is the length of the principal-diagonal vector of  $A^T A$  whose elements are  $q_{i,i}$  so that

$$q = \left( \sum_i q_{i,i}^2 \right)^{1/2} \quad (B8)$$

The number  $p$  is the length of a vector given by the matrix product  $B^T R$ , whose elements are  $p_i$ , so that

$$p = \left( \sum_i p_{i,i}^2 \right)^{1/2} \quad (B9)$$

The elements of  $B$  are second derivatives of the residual given by

$$b_{ij} = y_j^2 (\partial^2 R_i / \partial y_j^2) \quad (B10)$$

Finite differences are used to find  $a_{ij}$  and  $b_{ij}$ . First treat the profile parameter  $y_1$  as follows for all wavelengths:

- (a) Calculate current values of  $N_L$  and  $\tau_L$
- (b) Increase  $y_1$  by multiplying it by 1.01
- (c) Calculate new values  $N_{L,a}$  and  $\tau_{L,a}$
- (d) Decrease  $y_1$  by a factor 0.99/1.01
- (e) Calculate new values  $N_{L,b}$  and  $\tau_{L,b}$
- (f) Restore  $y_1$  to its starting value by multiplying it by 1/0.99

The first derivatives for the  $i$ th wavelength,  $j$ th parameter are

$$\left. \begin{aligned} a_{ij} &= ({}^cN_{L,b} - {}^cN_{L,a})/[0.02(1 - m_{N_L})] \\ a_{ij} &= ({}^c\tau_{L,b} - {}^c\tau_{L,a})/[0.02(1 - m_{\tau_L})] \end{aligned} \right\} \quad (B11)$$

the second derivatives are

$$\left. \begin{aligned} b_{ij} &= -({}^cN_{L,a} + {}^cN_{L,b} - 2{}^cN_L)/[0.01^2(1 - m_{N_L})] \\ b_{ij} &= -({}^c\tau_{L,a} + {}^c\tau_{L,b} - 2{}^c\tau_L)/[0.01^2(1 - m_{\tau_L})] \end{aligned} \right\} \quad (B12)$$

Next, repeat the procedure (steps (b) through (f)) for the succeeding profile parameters  $y_j$ .

## APPENDIX C

DETERMINATION OF  $\xi$  IN EQUATION (27)

The WAVES program involves the determination of how wavelength  $\lambda$  affects the relation between a dependent temperature profile parameter  $Z$  and an independent temperature-profile parameter  $w$ . At the initial value  $w_0$ , the value of  $Z(w_0)$  is invariant with wavelength. However,  $Z(w, \lambda)$  changes slightly with wavelength when  $w \neq w_0$ . The temperature-profile determination depends on these small changes. A graph of  $Z$  against  $w$  on an ordinary sheet of graph paper would show curves of considerable slope, so that differences between curves for various values of  $\lambda$  would not be readily apparent. To exaggerate these differences, the ordinate is changed from  $Z$  to  $Z + \xi(w - w_0)$ . The value of  $\xi$  is determined as follows.

Let the range of the independent parameter be

$$w_n \leq w \leq w_m$$

Among the values of  $Z(w)$  for all the wavelengths which are tried in the computation, there will be a maximum value  $Z_{\max}(w_n)$  and a minimum value  $Z_{\min}(w_n)$ . Similarly, there will be a maximum value  $Z_{\max}(w_m)$  and a minimum value  $Z_{\min}(w_m)$ . The value of  $\xi$  is taken as

$$\xi = \frac{1}{2} \left[ \frac{Z_{\max}(w_n) + Z_{\min}(w_n)}{2(w_n - w_0)} + \frac{Z_{\max}(w_m) + Z_{\min}(w_m)}{2(w_m - w_0)} \right] \quad (C1)$$

The total span of ordinate values is thereby reduced severalfold.

## APPENDIX D

## PROFIL PROGRAM

## Program Symbols

The following FORTRAN symbol list includes symbols in the sub-routines of appendixes E and F. It does not include symbols defined for NAMELIST and READ data in the section PROFIL PROGRAM USE.

<u>FORTRAN symbol</u>	<u>Description</u>
A(5, 5)	Condensed matrix of first derivatives
B(4)	Condensed matrix of second derivatives
BB(8, 3, 41)	Denormalized and broadened BO
BE(8, 3, 41)	BB weighted by KK
BO(8, 3, 21)	Interpolated local value of BTAB
CP(6, 41)	Constant of pressure profiles; ratio of each absorbing gas pressure to first absorbing gas pressure; ratio of each nonabsorbing gas pressure to the total pressure of non-absorbing gases
C1	Constant of pressure profile of first absorbing gas, $PW(1)/PC(1)$
DAMP	Damping constant for diagonal of least squares matrix
DEL(4)	Fractional change of variable parameter for derivatives (in data statement)
DPA(4)	Variable parameter increment for iteration step
DPAPA(4)	Fractional value of DPA

<u>FORTTRAN symbol</u>	<u>Description</u>
DPV(3)	DPA in condensed matrix
DTAU(8, 41)	Increment in transmittance
DUM	Dummy to prevent overflow or underflow
DUM1	Dummy to prevent overflow or underflow
DUM2	Dummy to prevent overflow or underflow
DX(41)	Distance between stations X along path
ERR(10)	Residual caused by errors ERRV and ERRK
ETA(8, 3, 41)	Interpolation parameter
G(10, 6)	First derivatives for least squares matrix
GSAV(8, 4)	Dummy variable equal to G
GV(9, 5)	Dummy variable equal to G in condensed matrix
H(9, 5)	Second derivatives for damping least squares matrix
HV(9, 5)	Dummy variable equal to H
IA	Index parameter equal to I
IB	Index parameter equal to I1
ITER1	Iteration counter
I2	Wavenumber index parameter I+1
JMIR	Index for reflection of profile about center
J2	Path index parameter (J1+1)/2
J3	Path index parameter J1+1
KO(8, 3, 21)	Interpolated local value of KTAB
KEY	Selector for variable parameters

<u>FORTTRAN symbol</u>	<u>Description</u>
KEY1(8)	Index parameter (data statement)
KEY2(8)	Index parameter (data statement)
KEY3(8)	Index parameter (data statement)
KK(8, 3, 41)	Denormalized KO
KV	Index of condensed matrix
KV2	Index parameter KV+2
K1	Index parameter for variable parameters
K2	Index parameter for variable parameters
K3	Index parameter for variable parameters
LX	Index parameter for error array
L3	Index parameter for gas type
MAX	Largest absolute value of all DPAPA for an iteration step
NEWLIM	Controls number of tests for upper and low parameter limits
NP1	Equals pressure profile equation exponent NP(1)
NTEST	Diagnostic indicator of absorbing gas pressure being greater than static
P(6, 41)	Pressure of each gas at each station along path
PAERR(4, 10)	Error of variable parameter caused by a residual ERR
PA1(4)	Tentative value of new PA for an iterative step
PSUM	Sum of pressure of all absorbing gases along path



<u>FORTRAN symbol</u>	<u>Description</u>
R(8, 41)	Gas radiance
RA(8)	Equals CRL during numerical differentiation
RAB(8)	Equals CRL before numerical differentiation
RB(8)	Equals CRL during numerical differentiation
R1(8)	Constant of Planck equation
R2(8)	Constant of Planck equation
STEP	Sum of fractional changes to variable parameters for an iteration step
T(41)	Temperature at each station along path
TAU(8, 4, 41)	Transmittance at each station along path
U(8, 3, 41)	Optical depth at each station along path
WAVOUT(10)	Wavenumbers in sequence for printout
X(41)	Actual path lengths $Z \cdot \text{PATH}/2$
Y(21)	Dummy equal to Z, the normalized path length

## PROFILE Program Listing

```

00101 1*      CC4404 PROF,TWB, L1,J1,J2,J3,C1,PSUM,JB,R1(R),R2(R),X(41),
00102 2*      X PA(4),CTAUL(8),CRL(8),T(41),DX(41),VK,VF,PS,PATH,L2, Y(21),L3,
00103 3*      X DTAUL(R,41),R(6,41),CP(6,41),P(6,41),ALPH(3,8),
00104 4*      X T4TAR( 8),KTAR(8,3,8),KQ(R,3,21),KK(9,3,41),TBTAR(8),
00105 5*      X BTAB(8,3,8),BO(6,3,21),KP(8,3,41),RE(8,3,41),ETA(8,3,41),
00106 6*      X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST,TX
00107 7*      REAL KK,KTAB,KQ,NP1
00108 8*      INTEGER PROF,DONE
00109 9*      DIMENSION DPAPA(4),RAR(R),DPA(4),KEY1(8),KEY2(8),KEY3(8),DEL(4),
00110 10*     X RA(8),RB(8),E(4),DPV(3),PA1(4),BOTLIM(4),UPLIM(4),LIM(4),MRL(8),
00111 11*     X MTAUL(R),G(10,6),H(9,5),GV(9,5),HV(9,5),A(5,5),PAERR(4,10)
00112 12*     X ,SAS(6),WAVE(6),Z(21),ERR(10),WAVOUT(10),GSAV(R,4),PW(6),NP(4),
00113 13*     X PC(6)
00114 14*     REAL MTAUL,MRL,NT,NP,MAX
00115 15*     NAME LIST/NAME/MODE,PROF,IREAD,PATH,I1,WAVE,MRL,MTAUL,
00116 16*     X ERRV,ERRK,TW,TC,NT,TWB,JB,UPLIM,ROTLIM,L1,L2,PS,PC,NP,PW,NK,
00117 17*     X TKTAB,NB,TBTAB,J1,2,ITER,TX
00118 18*     DATA KEY1/4*1,2,2,3,0/,KEY2/3,2,3,1,3,2,3,0/,KEY3/1,1,2,4*1,0/
00119 19*     X ,DEL/4*.01/,J1/21/,Z/0.,.01,.02,.05,.1,.2,.3,.4,.5,.7,1.,10*1./
00120 20* 600 IFEAD=0
00121 21* READ(5,NAME,END=999)
00122 22* IF(IREAD.FQ.DIGO TO 67
00123 23* READ(5,8C)(GAS(I),L=1,6)
00124 24* READ(5,R1)((ALPH(L,LL),LL=1,8 ),L=1,L1)
00125 25* READ(5,P1)((KTAB(I,L,N),N=1,P),I=1,I1),L=1,L1)
00126 26* READ(5,R1)((RTAB(I,L,N),N=1,P),I=1,I1),L=1,L1)
00127 27* DO 65 L=1,L1
00128 28* ALPH(L,L)=1.
00129 29* DO 66 I=1,I1
00130 30* DO 68 N=1,NK
00131 31* 65 IF(KTAB(I,L,N).LT. .1E-06)KTAB(I,L,N)=.1E-06
00132 32* DO 66 N=1,NB
00133 33* 66 IF(RTAB(I,L,N).LT. .1E-06)RTAB(I,L,N)=.1E-06
00134 34* 67 CONTINUE
00135 35* WRITE(6,90)
00136 36* WRITE(6,NAME)

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00224 37*      IF(1WFAP,FO,3)GO TO 632
00225 38*      WRITE(6,87) (GAS(L),L=1,6)
00226 39*      WRITE(6,87) ((ALPHIL,LL),LL=1,8),L=1,L1)
00227 40*      WRITE(6,87) ((KTAP(1,L,N),N=1,8),I=1,11),L=1,L1)
00228 41*      WRITE(6,87) ((BTAB(I,L,N),N=1,8),I=1,11),L=1,L1)
00229 42*      C      INITIAL CONDITIONS
00230 43*      VTEST=0
00231 44*      500 I=1
00232 45*      IH=I1
00233 46*      DCNE=0
00234 47*      ITER=0
00235 48*      DAMP=0.
00236 49*      I2=I1+1
00237 50*      J3=J1+1
00238 51*      J2=(J1+1)/2
00239 52*      L3=L1+1
00240 53*      C1=PW(1)/PC(1)
00241 54*      PA(1)=VT
00242 55*      PA(2)=TC
00243 56*      PA(3)=PC(1)
00244 57*      PA(4)=TW
00245 58*      DO 64 K=1,4
00246 59*      DPAPA(K)=0.
00247 60*      DPA(K)=0.
00248 61*      CTAUL(K)=0.
00249 62*      CTAUL(K+1)=0.
00250 63*      DO 64 I=1,10
00251 64*      WAVEOUT(I)=0.
00252 65*      ERR(I)=0.
00253 66*      S(I,K)=0.
00254 67*      S(I,S)=0.
00255 68*      64 PAERR(X,I)=0.
00256 69*      DO 50 I=1,11
00257 70*      IF(MODE.EQ.1)GO TO 65
00258 71*      WAVEOUT(I)=WAVE(I)
00259 72*      WAVEOUT(I2)=WAVE(I1)
00260 73*      65 R1(I)=.11909(-11)*WAVE(I)**3
00261 74*      51 R2(I)=1.4788*WAVE(I)
00262 75*      DO 51 J=1,J2
00263 76*      JMIP=J3-J
00264 77*      X(J)=PATH*Z(J)/P.
00265 78*      Y(J)=Z(J)
00266 79*      51 X(JMIP)=PATH-X(J)
00267 80*      DO 55 J=2,J1
00268 81*      59 DX(J)=X(J)-X(J-1)
00269 82*      C      PRESSURE PROFILE INITIAL PROFILES
00270 83*      VF1=NP(1)
00271 84*      DO 52 J=1,J2
00272 85*      DO 53 L=1,L2
00273 86*      DUM1=ARS(PC(L)-PW(L))
00274 87*      P(L,J)=PC(L)
00275 88*      IF(DUM1.EQ.0.0D0,J.EQ.J2)GO TO 53
00276 89*      DUM=1.-V(J)
00277 90*      DUM2=ALOG(DUM1)+ALOG(DJ)/NP(L)
00278 91*      IF(DUM2.LT. -F0.)GO TO 53
00279 92*      58 P(L,J)=PC(L)-(PC(L)-PW(L))*DUM**((1./VF(L))
00280 93*      53 CONTINUE
00281 94*
00282 95*
00283 96*
00284 97*
00285 98*
00286 99*
00287 00*
00288 01*
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00403  94*      IF(L1.EQ.1)GO TO 55
00403  95*      C PRESSURE PROFILE RATIO FACTORS CP(L,J)
00403  96*      DO 54 L=2,L1
00410  97*      F4 CP(L,J)=P(L,J)/P(1,J)
00412  98*      F5 IF(L2.FQ.L1)GO TO 52
00414  99*      SUM=0.
00415  100*      DO 56 L=L2,L2
00420  111*      F6 SUM=SUM+P(L,J)
00422  112*      DO 57 L=L3,L2
00425  113*      F7 CP(L,J)=P(L,J)/SUM
00427  114*      F8 CONTINUE
00431  115*      IF(MODE.EQ.2)GO TO 701
00433  116*      CALL TEMP
00434  117*      CALL TRANS
00435  118*      DO 63 I=1,I1
00440  119*      MPL(I)=CPL(I)
00441  110*      F3 MTAUL(I)=CTAUL(I)
00443  111*      IF(MODE.EQ.1)GO TO 701
00445  112*      MODE=2
00446  113*      GO TO 600
00447  114*      701 WRITE(6,91)(PA(I),I=1,4),PW(1),NP(1)
00447  115*      C RESIN ITERATION LOOP
00447  116*      700 CALL TEMP
00447  117*      CALL TRANS
00447  118*      IF(NTEST.FQ.1)WRITE(6,77)
00447  119*      NTEST=0
00461  120*      C FIND RESIDUALS, TEST FOR SOLUTION OR MAXIMUM ITERATION NUMBER
00462  121*      RESID=0.
00463  122*      TAJAR=CTAUL(1)
00464  123*      DO 1 I=1,I1
00467  124*      PAR(I)=CPL(I)
00470  125*      S(I,5)=CPL(I)/MPL(I)-1.
00471  126*      1 RESID=RESID+G(I,5)**2
00473  127*      IF(MODE.EQ.1)GO TO 406
00475  128*      S(I2,5)=(MTAJUL(1)-CTAUL(1))/(1.-MTAJUL(1))
00475  129*      RESID=SQRT(RESID+G(I2,5)**2)
00477  130*      STEP=0.
00480  131*      DO 2 J=1,7,2
00483  132*      STEP=STEP+ABS(OPAPA(J))*1
00484  133*      2 STEP=STEP+ABS(OPAPA(J+1))
00486  134*      IF((ITER1.NT.0).AND.(STEP.LT..JDD1.OR.ITER1.EQ.ITER.OR.RESID.LT.
00490  135*      X .JDD1))GONE=1
00491  136*      WRITE(6,52)(OPA(I),I=1,4),ITER1,RESID,STEP,(PA(I),I=1,4),
00491  137*      X (S(I,5),I=1,5),(WAVOUT(I),I=1,5)
00491  138*      ITER1=ITER1+1
00491  139*      C DERIVATIVES EQ(11, 312)
00492  140*      406 KFY=1
00492  141*      41=KEY1(KFY)-1+PROF
00492  142*      42=KFY2(KEY)-1+PROF
00492  143*      43=KEY3(KFY)
00492  144*      DEL(1)=D1/PA(1)
00492  145*      DO 3 K=41,K2,K3
00492  146*      PA(K)=PA(K)*(1.+DEL(K))
00492  147*      CALL TEMP
00492  148*      CALL TRANS
00492  149*      DO 4 I=1,I1
00492  150*      4 PA(I)=CPL(I)
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10542 151*      TAU=CTAU(I)
10543 152*      PA(K)=PA(K)*(1.-DEL(K))/(1.+JFL(K))
10544 153*      CALL TEMP
10545 154*      CALL TRANS
10546 155*      DO 5 J=1,I1
10547 156*      5 RF(I)=CR(I)
10548 157*      TAU=CTAU(I)
10549 158*      PA(K)=PA(K)/(1.-DEL(K))
10550 159*      DO 6 J=1,I1
10551 160*      6 G(I,K)=(PA(I)-PB(I))/(2.*DEL(K)*MHL(I))
10552 161*      6 SAV(I,K)=G(I,K)
10553 162*      4 H(I,K)=(PA(I)+PB(I)-2.*PAR(I))/(DEL(K)*M2*MHL(I))
10554 163*      4 G(I2,K)=(TAU1-TAU2)/(2.*DEL(K)*(1.-MTAU(I)))
10555 164*      4 H(I2,K)=(TAU1+TAU2-2.*TAU2H)/(DEL(K)*M2*(1.-MTAU(I)))
10556 165*      3 CONTINUE
10557 166*      CALL TEMP
10558 167*      CALL TRANS
10559 168*      NEWLIM=7
10560 169*      DO 32 K=1,4
10561 170*      PA(K)=PA(K)
10562 171*      72 LIM(K)=0
10563 172*      C FOR MODE=1, SEQUENTIALLY SHIFT DERIVATIVES ABOVE I=2 TO I=2
10564 173*      DO 401 M1=2,I1
10565 174*      IF(MODE.NE.1)GO TO 500
10566 175*      I2=3
10567 176*      WAVEOUT(1)=WAVE(I1)
10568 177*      WAVEOUT(2)=WAVE(M1)
10569 178*      WAVEOUT(3)=WAVE(I1)
10570 179*      DO 402 K=K1,K2,K3
10571 180*      313,K)=G(I1+1,K)
10572 181*      402 G(I2,K)=GSAV(M1,K)
10573 182*      500 CONTINUE
10574 183*      C CHANGE DERIVATIVE VARIABLES TO CONDENSE ARRAY K=K1,K2,K3 TO K=1,KV
10575 184*      KV=0
10576 185*      DO 7 K=K1,K2,K3
10577 186*      KV=KV+1
10578 187*      DO 7 J=1,I2
10579 188*      6V(I,KV)=G(I,K)
10580 189*      7 HV(I,KV)=H(I,K)
10581 190*      C LEAST SQUARES MATRIX AT--A EQ(16)
10582 191*      DO 8 I=1,KV
10583 192*      DO 8 K=1,KV
10584 193*      A(I,K)=0.
10585 194*      DO 8 J=1,I2
10586 195*      8 A(I,K)=A(I,K)+G(V(J,K))*G(V(J,I))
10587 196*      IF(MODE.EQ.1)GO TO 403
10588 197*      C RESIDUAL VECTOR BT--R EQ(16) AND DAMPING VECTOR D EQ(16)
10589 198*      KV2=KV+2
10590 199*      DO 9 K=1,KV
10591 200*      A(K,KV2)=0.
10592 201*      B(K)=0.
10593 202*      DO 9 J=1,I2
10594 203*      A(K,KV2)=A(K,KV2)-G(V(J,K))*G(V(J,5))
10595 204*      9 B(K)=B(K)+HV(J,K)*G(V(J,5))
10596 205*      DAMP=7.
10597 206*      IF(I2.EQ.KV.OR.DONE.EQ.1)GO TO 12
10598 207*      C NORMALIZED DAMPING VECTOR P/L EQ(18, 19) AND DAMPED MATRIX

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00675 208*      D1=D.
00676 209*      D2=D.
00677 210*      DO 10 K=1,KV
00702 211*      D1=D1+A(K,K)*W
00703 212*      10 D2=D2+R(K)*W
00705 213*      DAMP=SQRT(D2/D1)
00706 214*      DO 11 K=1,KV
00711 215*      11 A(K,K)= A(K,K)*(1.+DAMP)
00713 216*      12 CONTINUE
00713 217*      C INVERSE OF LEAST SQUARES MATRIX AT--A
00714 218*      403 NV=KV+1
00715 219*      DO 13 I=1,KV
00720 220*      DO 14 J=1,KV
00723 221*      14 A(J,NV)=D.
00725 222*      A(I,NV)=1.
00726 223*      DIV=A(I,I)
00727 224*      DO 15 J=1,NV
00732 225*      15 A(I,J)= A(I,J)/DIV
00734 226*      DO 16 J=1,KV
00737 227*      IF(I.NE.J)GO TO 16
00741 228*      FAC=A(I,I)
00742 229*      DO 17 K=1,NV
00745 230*      17 A(J,K)=A(J,K)-A(I,K)*FAC
00747 231*      16 CONTINUE
00751 232*      DO 18 J=1,KV
00754 233*      18 A(J,I)=A(J,NV)
00756 234*      13 CONTINUE
00760 235*      IF(DONE.EQ.1.OR.MODE.EQ.1) GO TO 404
00763 236*      C SOLVE FOR PARAMETER FRACTIONAL INCREMENTS A-INVERSE*AT--R
00765 237*      DO 19 I=1,KV
00766 238*      DPV(I)=D.
00771 239*      DO 19 K=1,KV
00771 240*      19 DPV(I)=DPV(I)+A(I,K)*A(K,KV2)
00771 241*      C EXPAND INDEX TO ORIGINAL PARAMETER INDEX K=K1,K2,K3
00774 242*      4V=7
00775 243*      DO 20 K=K1,K2,K3
00801 244*      NV=KV+1
00802 245*      DPAPA(K)=DPV(KV)
00802 246*      20 DPA(K)= DPAPA(K)*PA(K)
00802 247*      C PROPORTIONALLY REDUCE PARAMETER STEP SIZE FOR LARGEST STEP .1*PA
00802 248*      C OR .1 FOR PA(1)
00804 249*      MAX=D.
00805 250*      DO 21 K=K1,K2,K3
00810 251*      DUM=ABS(DPA(K))
00811 252*      IF(K.NE.1)DUM=DUM/PA(1)
00815 253*      21 IF(DUM.GT.MAX)MAX=DUM
00816 254*      IF(MAX.LT.1)MAX=.1
00820 255*      DO 22 K=K1,K2,K3
00823 256*      22 PA(K)=PA(K)+DPA(K)*.1/MAX
00823 257*      C TEST FOR TENTATIVE PARAMETERS OUTSIDE LIMIT
00825 258*      DO 23 K=K1,K2,K3
00830 259*      K4=K+1-PROF
00831 260*      IF(PA(K).GE.ROTLIM(K))GO TO 24
00833 261*      PA(K)=ROTLIM(K)
00834 262*      WRITE(6,83)K,PA(K)
00840 263*      14(K4)=1
00841 264*      24 IF(PA(K).LE.UPLIM(K))GO TO 23

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PA1(K)=DPLIM(K)
WRITE(6,*,7X,PA1(K))
LIM(K)=1
27 CONTINUE
NEWLIM=NEWLIM+1
IF(NEWLIM.EQ.2) GO TO 28
KEY=1+4*(LIM(1)+2*LIM(2)+LIM(3))
L1=KEY1(KEY)-1+DOWF
L2=KEY2(KEY)-1+DOWF
L3=KEY3(KEY)
IF(KEY.FW.1.OR.KEY.EQ.4) GO TO 26
GO TO 29
ACCEPT LIMITS AND TENTATIVE PARAMETERS
26 DO 27 K=1,4
DPA(K)=PA1(K)-PA(K)
DPA(K)=DPA(K)/PA(K)
27 PA(K)=PA1(K)
GO TO 700
PARAMETER ERROR ESTIMATE
404 DO 23 I=1,11
23 ERR(I)=SQRT(1+.2*CTAUL(I)/(1.-CTAUL(I)))*ERRV
ERR(I)=CTAUL(I)/(1.-CTAUL(I))*SQRT(2.*ERRV**2+(ALOG(CTAUL(I))
X *ERRK)**2)
IF(MODE.NE.1) GO TO 34
ERR(2)=SQRT(1+.2*CTAUL(H1)/(1.-CTAUL(H1)))*ERRV
ERR(4)=0.
ERR(5)=0.
ERR(6)=0.
34 DO 24 L=1,3
LX(L)=1+DOWF
PAERR(LX,L)=0.
DO 25 J=1,12
PAERR(LX,J)=0.
DO 31 K=1,3
JLX=1+DOWF
31 PAERR(LX,I)=PAERR(LX,I)+A(L,K)*S(I,J)*ERR(I)
32 PAERR(LX,K)=PAERR(LX,K)+PAERR(LX,I)*S(I,K)
33 PAERR(LX,K)=SQRT(PAERR(LX,K))
PSUM=0.
DO 35 L=1,11
35 PSUM=PSUM+P(L,J)
IF(PSUM.GT.95) WRITE(6,77)
WRITE(6,*,4) (IPAR(L,I),L=1,4),WAVOUT(T),ERR(I),I=1,6)
401 IF(MODE.NE.1) GO TO 407
407 CONTINUE
WRITE(6,30)(WAVE(I),I=1,8),(CTAUL(I),I=1,9),(GAS(L),L=1,6),
X (X(J),J=1),(P(I,J),I=1,6),J=1,3)
GO TO 600
71 FORMAT (50H A SCORING GAS PRESSURE GREATER THAN STATIC PRESSURE )
81 FORMAT(A6F)
91 FORMAT ( 3F6.0)
92 FORMAT (1H/1HD,14HINCREMENTS DPA ,F9.5,F9.2,F9.5,F9.2,4X,
X 10HITERATIONS ,12,7X,14HMS RESIDUAL= ,E3.3,7H STEPS= ,E9.3
X /1HD,14HPARAMETERS PA ,F9.5,F9.2,F9.5,F9.2,4X,
X 14HRESIDUALS= ,F10.3/4X,17HWAVENUM= ,F(1/CM)= ,5F10.0)
93 FORMAT (1HD,17HLIMIT REACHED,PA(1,1,2H)= ,F9.3)
94 FORMAT (1HD/ 1X,15HPARAMETER ERROR,3F8.3,15HWAVENUMHER (1/CM),2X,
X 15HRESIDUAL PERCENT,1X,14HPERCENT ,7X,4(F8.1,1HX),F11.2,9X,4(F8.1,1HX
X /415X,4F9.1,F10.2, 9X,F8.1/16X,9HMS TOTAL ,4F9.1,F10.0, 9X,F8.1)
95 FORMAT (1HD,5HBASE= ,4(1X,A6))
96 FORMAT (1HD,5HLPD= ,4F10.2/16X,4F10.2))
97 FORMAT (1HD,5HKTAK= ,4F10.4/16X,4F10.4))
98 FORMAT (1HD,5HETAK= ,4F10.7/16X,4F10.3))
99 FORMAT (1H)
91 FORMAT (1H,7X,7HPROFILE,5X,4HTEMP,4X,5HAXIAL,4X,5HAXIAL,5X,4HWALL,
X 15X,4HWALL,4X,5HPERCENT,10HPARAMETERS,7X,5HEXPONENT,3X,4HTEMP,4X,
X 5HPERCENT,5X,4HTEMP,14X,5HPERCENT,3X,4HEXPONENT/21X,2HNT,4X,4HTEMP,4X,
X 5HTEMP,4X,4HTEMP,4X,6HTEMP,4X,2HTEMP/17X,F9.5,F9.2,F9.5,F9.2,
X 9X,2F9.5)
31 FORMAT (1H,15HWAVENUMHER (1/CM)= ,4F9.7/16H TRANSMITTANCE= ,
X 4F9.3/ 1HD,19HTEMPERATURE PROFILE, 5X,14HPARTIAL PRESSURE PROFILE,5
X 14H GAS,ATM /4X,4HX,CM,4X,4HTEMP,K ,5(7X,16G)/13(1X,F7.2,F10.2
X ,F9.4/11X))
999 STOP
END

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## APPENDIX E

## TEMP SUBROUTINE LISTING

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C0101 1*      SUBROUTINE TEMP                                C00012
C0102 2*      COMMON PROF,TWB, L1,J1,J2,J3,C1,PSUM,JB,R1(8),R2(8),X(41), C00012
C0103 3*      X PA(4),CTAUL(8),CPL(8),T(41),DX(41),NK,NB,PS,PATH,L2, Y(21),L3, C00012
C0104 4*      X LTAU(8,41),R(8,41),CP(6,41),P(6,41),ALPH(3,8), C00012
C0105 5*      X XTAB( 8),KTAB(8,3,8),KO(8,3,21),KK(8,3,41),TBTAB(8), C00012
C0106 6*      X PTAB(8,3,8),PD(8,3,21),PB(8,3,41),BE(8,3,41),ETA(8,3,41), C00012
C0107 7*      X U(8,3,41),TAU(8,4,41),NP1,IA,IB,NTEST,TX C00012
C0108 8*      REAL KK,KTAB,KO,NP1 C00012
C0109 9*      INTEGER PROF C00012
C0110 10*      C TEMP AND PRINCIPAL PRESSURE PROFILE EQ(1,2,3) C00012
C0111 11*      PW1=PA(3)*C1 C00012
C0112 12*      DUM1=ARS(PA(2)-PA(4)) C00031
C0113 13*      DUM2=ARS(PA(3)-PW1) C00037
C0114 14*      DO 1 J=1,J2 C00042
C0115 15*      JMIR=J3-J C00056
C0116 16*      T(J)=PA(2) C00061
C0117 17*      DUM4=-Y(J) C00063
C0118 18*      IF(DUM1.EQ.0..OR.J.EQ.J2)GO TO 11 C00066
C0119 19*      DUM3=ALOG(DUM1)+ALOG(DUM)/PA(1) C00075
C0120 20*      IF(DUM3.LT.-8C)GO TO 2 C00107
C0121 21*      11 T(J)=PA(2)-(PA(2)-PA(4))*DUM**(1./PA(1)) C00113
C0122 22*      2 IF(Y(J).GT. .51) T(J)=T(J)+TX*(SIN(3.1416*(Y(J)-.5)))*2 C00122
C0123 23*      T(JMIR)=T(J) C00142
C0124 24*      P(1,J)=PA(3) C00145
C0125 25*      IF(DUM2.EQ.0..OR.J.EQ.J2)GO TO 1 C00147
C0126 26*      DUM3=ALOG(DUM2)+ALOG(DUM)/NP1 C00156
C0127 27*      IF(DUM3.LT.-8C)GO TO 1 C00170
C0128 28*      12 P(1,J)=PA(3)-(PA(3)-PW1 )*DUM**(1./NP1) C00173
C0129 29*      1 P(1,JMIR)=P(1,J) C00203
C0130 30*      C PRESSURE PROFILE OF OTHER ABSORBING GASES C00210
C0131 31*      DO 3 J=1,J2 C00224
C0132 32*      JMIR=J3-J C00231
C0133 33*      PSUM=. C00232
C0134 34*      IF(L1.EQ.1)GO TO 4 C00234
C0135 35*      DO 5 L=L2,L1 C00244
C0136 36*      P(L,J)=P(1,J)*CP(L,J) C00246
C0137 37*      P(L,JMIR)=P(L,J) C00247
C0138 38*      5 PSUM=PSUM+P(L,J) C00254
C0139 39*      4 PSUM=PSUM+P(1,J) C00254
C0140 40*      C PRESSURE PROFILE OF NON ABSORBING GASES C00264
C0141 41*      IF(L2.EQ.L1)GO TO 3 C00267
C0142 42*      DUM=PS-PSUM C00276
C0143 43*      IF(DUM.LT.0.)DUM=0. C00276
C0144 44*      DO 7 L=L3,L2 C00310
C0145 45*      P(L,J)=DUM*CP(L,J) C00310
C0146 46*      7 P(L,JMIR)=P(L,J) C00312
C0147 47*      3 IF(PSUM.GT.PS)NTEST=1 C00316
C0148 48*      C TEMPERATURE BOUNDARY LAYER,WALL TEMPERATURE TWB C00316
C0149 49*      IF(JB.LE.1..OR.PROF.EQ.1)GO TO 9 C00327
C0150 50*      DO 8 J=1,JB C00344
C0151 51*      JMIR=J3-J C00356
C0152 52*      DUM=(T(J2)-T(JB))/(PA(1)*(1.-Y(JB))) C00361
C0153 53*      DUMD=Y(J)/Y(JB) C00366
C0154 54*      T(J)=TWB+(T(JR)-TWB)*DUM+(DUM*Y(JB)+TWB-T(JB))*DUM*(DUMD-1.) C00371
C0155 55*      8 T(JMIR)=T(J) C00406
C0156 56*      C RADIANCE PROFILE FOR I WAVELENGTHS,PLANCK FUNCTION C00412
C0157 57*      DO 10 J=1,J2 C00420
C0158 58*      JMIR=J3-J C00423
C0159 59*      DO 10 I=1A,IB C00433
C0160 60*      DUM=R2(I)/T(J) C00436
C0161 61*      IF(ABS(DUM).GT.RD.)DUM=PJ. C00443
C0162 62*      R(I,J)=R1(I)/(EXP(DUM)-1.) C00452
C0163 63*      10 R(I,JMIR)=R(I,J) C00462
C0164 64*      RETURN C00462
C0165 65*      END C00462

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## APPENDIX F

## TRANS SUBROUTINE LISTING

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00171 1*      SUBROUTINE TRANS
00172 2*      COMMON PROF,TWR, L1,J1,J2,J3,C1,PSUM,JB,R1(R),R2(R),X(41),
00173 3*      X PA(4),CTAUL(R),CRL(8),T(41),TX(41),VK,NB,PS,PATH,L2, Y(21),L3,
00174 4*      X TAU(JP,41),R18(41),CP(6,41),P(6,41),ALPH(3,8),
00175 5*      X TKTAR( 8),KTAR(8,3,R),KC(R,3,21),KK(8,3,41),TBTAB(8),
00176 6*      X ETAB(8,3,8),BC(8,3,21),BR(8,7,41),RE(8,3,41),ETA(8,3,41),
00177 7*      X U(R,7,41),TAU(P,4,41),NP1,IA,IB,NTEST,7X
00178 8*      REAL KK,KTAR,KC,NP1
00179 9*      INTEGER PROF
00180 10*      DIMENSION BBETAP(7),A1(7),A2(7),A3(7),A4(7)
00181 11*      DATA BBETAP/D.,2.,5.,10.,20.,50.,100./,A1/-68,-37,.60,3.19,9.13,
00182 12*      X 29.1,105./,A2/-35,.62,3.15,9.25,22.8,67.1,209./,A3/.55,.71,.97,
00183 13*      X 1.15,1.67,2.76,4.05/,A4/.07,.43,.79,1.30,2.26,4.56,7.09/
00184 14*      C RAND MODEL PARAMETER PROFILE BY TABULAR INTERPOLATION
00185 15*      DO 1 I=IA,IB
00186 16*      DO 1 L=1,L1
00187 17*      DO 2 J=1,J2
00188 18*      JMIR=J3-J
00189 19*      C INTERPOLATE FOR KC AND BC, DENORMALIZE KC TO KK, EQ(14.1)
00190 20*      DO 3 N=2,NK
00191 21*      IF(T(J).GT.TKTAR( N).AND.N.NE.NK)GO TO 3
00192 22*      KC(I,L,J)=KTAB(I,L,N-1)+(KTAB(I,L,N)-KTAB(I,L,N-1))
00193 23*      X*(T(J)-TKTAR( N-1))/(TKTAR( N)-TKTAR( N-1))
00194 24*      IF(T(J).LT.TKTAR(1))KC(I,L,J)=KTAR(I,L,1)
00195 25*      IF(T(J).GT.TKTAR(NK))KC(I,L,J)=KTAB(I,L,NK)
00196 26*      GO TO 4
00197 27*      3 CONTINUE
00198 28*      4 KC(I,L,J)=KC(I,L,J)*273.*P(L,J)/T(J)
00199 29*      2 KC(I,L,JMIR)=KK(I,L,J)
00200 30*      C INTERPOLATE FOR BC
00201 31*      DO 1 J=1,J2
00202 32*      DO 5 N=2,NB
00203 33*      IF(T(J).GT.TBTAB( N).AND.N.NE.NB)GO TO 5
00204 34*      BC(I,L,J)=BTAB(I,L,N-1)+(BTAB(I,L,N)-BTAB(I,L,N-1))
00205 35*      X*(T(J)-TBTAB( N-1))/(TBTAB( N)-TBTAB( N-1))
00206 36*      IF(T(J).LT.TBTAB(1))BC(I,L,J)=BTAB(I,L,1)
00207 37*      IF(T(J).GT.TBTAB(NB))BC(I,L,J)=BTAB(I,L,NB)
00208 38*      GO TO 1
00209 39*      5 CONTINUE
00210 40*      1 CONTINUE
00211 41*      C LINE BROADENING AND DENORMALIZE BC TO BR EQ(14.2)
00212 42*      DO 6 J=1,J2
00213 43*      JMIR=J3-J
00214 44*      DO 6 L=1,L1
00215 45*      DUM=0.
00216 46*      DO 7 LL=1,L2
00217 47*      7 DUM=DUM+ALPH(LL)*P(LL,J)
00218 48*      DO 6 I=IA,IB
00219 49*      3B(I,L,J)=RO(I,L,J)*DUM
00220 50*      6 3B(I,L,JMIR)=3B(I,L,J)
00221 51*      C 3E EQ(17)
00222 52*      DO 8 I=IA,IB
00223 53*      DO 8 L=1,L1
00224 54*      3E(I,L,1)=3B(I,L,1)
00225 55*      S1=0.
00226 56*      S2=0.
00227 57*      SAV1=KK(I,L,1)*PB(I,L,1)
00228 58*      DO 8 J=2,J1
00229 59*      SAV2=KK(I,L,J)*PB(I,L,J)
00230 60*      S1=S1+(KK(I,L,J-1)+KK(I,L,J))*DX(J)
00231 61*      S2=S2+(SAV1+SAV2)*DX(J)
00232 62*      SAV1=SAV2
00233 63*      RE(I,L,J)=S2/S1
00234 64*      8 CONTINUE
00235 65*      C OPTICAL DEPTH U EQ(11), AND ETA EOS(13),(14)
00236 66*      DO 9 I=IA,IB
00237 67*      DO 9 L=1,L1
00238 68*      ETA(I,L,1)=0.
00239 69*      J(I,L,1)=0.
00240 70*      S1=0.
00241 71*      SAV1=KK(I,L,1)

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00260      72*      DO 9 J=2,J1      000551
00263      73*      BBE=BR(I,L,J)/BF(I,L,J)      000551
00264      74*      IF(BBE.GT.100.)RBE=100.      000554
00266      75*      SAV2=KK(I,L,J)*RBE*ETA(I,L,J-1)      000562
00267      76*      S1=S1+(SAV1+SAV2)*DX(J)*.5      000572
00270      77*      SAV1=SAV2      000577
00271      78*      J(I,L,J)=S1/BE(I,L,J)      000601
00272      79*      DO 10 N=2,7      000606
00275      80*      IF(BBE.GT.BBETAB(N).AND.N.NE.7)GO TO 10      000606
00277      81*      RATIO=(BBE-BBETAB(N-1))/(BBETAB(N)-BBETAB(N-1))      000623
00300      82*      A5=1.+185*BBE      000631
00301      83*      IF(U(I,L,J).GT.A5)ETA(I,L,J)=(U(I,L,J)+A1(N-1)+(A1(N)-A1(N-1))      000635
00301      84*      X*RATIO)/(U(I,L,J)+(A2(N)-A2(N-1))*RATIO+A2(N-1))      000635
00303      85*      IF(U(I,L,J).LE.A5)ETA(I,L,J)=(U(I,L,J)*(A3(N-1)+(A3(N)-A3(N-1))      000656
00303      86*      X*RATIO)/(A5+U(I,L,J)*(A4(N)-A4(N-1))*RATIO+A4(N-1)))      000656
00305      87*      GO TO 11      000677
00306      88*      10 CONTINUE      000726
00310      89*      11 CONTINUE      000726
00311      90*      9 CONTINUE      000726
00311      91*      C      TAU FOR LI GASES, EQ (9),(10)      000726
00315      92*      DO 12 I=1A,1B      000726
00320      93*      DO 13 J=1,J1      000726
00323      94*      TAU(I,4,J)=1.      000726
00324      95*      DO 14 L=1,L1      000731
00327      96*      TAU(I,L,J)=EXP(-U(I,L,J)*BE(I,L,J)/SQRT(1.+1.5708*U(I,L,J)))      000731
00330      97*      14 TAU(I,4,J)=TAU(I,4,J)*TAU(I,L,J)      000751
00332      98*      13 CONTINUE      000766
00334      99*      12 CTAUL(I)=TAU(I,4,J)      000766
00334      100*      C      GAS RADIANCE CRL EQ (8)      000766
00336      101*      DO 15 I=1A,1B      001015
00341      102*      CRL(I)=0.      001017
00342      103*      DO 15 J=2,J1      001022
00345      104*      CTAU(I,J)=TAU(I,4,J-1)-TAU(I,4,J)      001022
00346      105*      15 CRL(I)=CRL(I)+(P(I,J)+R(I,J-1))*DTAU(I,J)*.5/(1.-CTAUL(I))      001024
00351      106*      RETURN      001045
00352      107*      END      001122

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## APPENDIX G

## WAVES PROGRAM

## Program Symbols

The following FORTRAN symbol list is limited to symbols not in the PROFIL symbol list, APPENDIX D, and not in the NAMELIST data in the section WAVES PROGRAM USE.

<u>FORTRAN SYMBOL</u>	<u>DESCRIPTION</u>
AMAX	Maximum value of dependent profile parameter to determine ZETA
AMIN	Minimum value of dependent profile parameter to determine ZETA
KEY	Selector for variable profile parameters, KEY=K <sup>4</sup> +PROF-1
KEY <sup>4</sup> (5)	Index parameter (data statement)
K5	Index parameter to select dependent variable profile parameter
NPB	Index parameter NPA-1
PASAV (8,10)	Dependent variable parameter after correction by ZETA
PASAVE (4)	Saves initial value of independent variable parameter
ZETA (11)	Graph-plotting constant (APPENDIX C)

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00277	45*	42=KEY2(KEY)	003374
00300	46*	43=KEY3(KEY)	000376
00301	47*	45=KEY4(KEY)	000400
00302	48*	VTES=0	000402
00303	49*	IA=1	000403
00304	50*	IB=1	000405
00305	51*	J3=J1+1	000407
00306	52*	J2=(J1+1)/2	000411
00307	53*	L3=L1+1	000413
00310	54*	C1=PW(1)/PC(1)	000415
00311	55*	PA(1)=NT	000420
00312	56*	PA(2)=YC	000422
00313	57*	PA(3)=PC(1)	000424
00314	58*	PA(4)=TM	000426
00315	59*	DO 64 K=1,4	000455
00320	60*	DPAPAK(K)=0.	000455
00321	61*	DPA(K)=0.	000455
00322	62*	PASAVE(K)=PA(K)	000456
00323	63*	DO 64 I=1,6	000464
00326	64*	G(K,I)=0.	000464
00327	65*	G(K+4,I)=0.	000464
00330	66*	G(I,I)=0.	000465
00331	67*	PASAVIK(I+4)=0.	000466
00332	68*	PASAVIK+4,I+4)=0.	000467
00333	69*	DO 64 M=1,4	000472
00336	70*	TAU(I+2,M,M)=0.	000472
00337	71*	TAU(I,M)=0.	000472
00340	72*	CP(I,M)=0.	000473
00341	73*	64 CONTINUE	000517
00345	74*	DO 50 I=1,I1	000517
00350	75*	R1(I)=.11909E-11 *WAVE(I)*3	000517
00351	76*	50 R2(I)=1.4388*WAVE(I)	000523
00353	77*	DO 51 J=1,J2	000532
00356	78*	JMIR=J3-J	000532
00357	79*	X(J)=PATH+Z(J)/2.	000535
00360	80*	Y(J)=Z(J)	000541
00361	81*	51 X(JMIR)=PATH-X(J)	000543
00363	82*	DO 59 J=2,J1	000553
00366	83*	59 DX(J)=X(J)-X(J-1)	000553
00366	84*	C PRESSURE PROFILE INITIAL PROFILES	000553
00370	85*	VP1=VP(1)	000556
00371	86*	DO 52 J=1,J2	000556
00374	87*	DO 53 L=1,L2	000605
00377	88*	DUM1=ABS(PC(L)-PW(L))	000605
00400	89*	P(L,J)=PC(L)	000610
00401	90*	IF(DUM1.EQ.0..OR.J.EQ.J2)GO TO 53	000612
00403	91*	DUM=1.-Y(J)	000617
00404	92*	DUM2=ALOG(DUM1)*ALOG(DUM1)/NP(L)	000621
00405	93*	IF(DUM2.LT. -.83.160 TO 53	000633
00407	94*	58 P(L,J)=PC(L)-(PC(L)-PW(L))*DUM*(1./VP(L))	000636
00410	95*	53 CONTINUE	000656
00412	96*	IF(L1.EQ.1)GO TO 55	000656
00412	97*	C PRESSURE PROFILE RATIO FACTORS CP(L,J)	000656
00414	98*	DO 54 L=2,L1	000660
00417	99*	54 CP(L,J)=P(L,J)/P(1,J)	000666
00421	100*	55 IF(L2.EQ.L1)GO TO 52	000672
00423	101*	DUM=0.	000674

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00424	102*	DO 56 L=L1,L2	000700
00427	103*	56 DUM=DUM+PIL,J)	000710
00431	104*	DO 57 L=L3,L2	000717
00434	105*	57 CPIL,J)=PIL,J)/DUM	000717
00436	106*	52 CONTINUE	000726
00440	107*	CALL TEMP	000726
00441	108*	CALL TRANS	000730
00442	109*	DO 63 I=1,I1	000732
00445	110*	MRL(I)=CRL(I)	000740
00446	111*	63 MTAUL(I)=CTAUL(I)	000741
00450	112*	WRITE(6,351)(GASIL,L=1,6),IX(J),Y(J),IP(I,J),I=1,6),J=1,J1)	000744
00464	113*	WRITE(6,90)	000770
00466	114*	WRITE(6,91)	000775
00466	115*	C INDEPENDENT VARIABLE PARAMETER PA(K4)	000775
00470	116*	DO 602 I=1,I1	001005
00473	117*	IA=I	001021
00474	118*	IB=I	001023
00475	119*	DO 602 IPA=1,NPA	001030
00503	120*	PA(K4)=PA1(IPA)	001030
00501	121*	ITER1=0	001032
00502	122*	I2=I+1	001033
00502	123*	C BEGIN ITERATION LOOP	001033
00503	124*	700 CALL TEMP	001036
00504	125*	CALL TRANS	001037
00505	126*	IF(NTST.EQ.1)WRITE(6,73)	001041
00510	127*	NTST=0	001051
00510	128*	C FIND RESIDUALS, TEST FOR SOLUTION OR MAXIMUM ITERATION NUMBER	001051
00511	129*	TAUAB=CTAUL(I)	001052
00512	130*	RAB(I)=CRL(I)	001054
00513	131*	G(I,5)=CRL(I)/MRL(I)-1.	001056
00514	132*	S(I,2,5)=(MTAUL(I)-CTAUL(I))/(1.-MTAUL(I))	001061
00515	133*	RESID=SQRT((CRL(I)/MRL(I)-1.)**2+(MTAUL(I)-CTAUL(I))/(1.-MTAUL(I))	001065
00515	134*	X )**2)	001065
00516	135*	IF((ITER1.GT.0).AND.(ITER1.EQ.ITER.OR.RESID.LT..0001))GO TO 604	001075
00520	136*	ITER1=ITER+1	001126
00520	137*	C DERIVATIVES EQ(R11 B12)	001126
00521	138*	DEL(I)=01/PA(I)	001131
00522	139*	DO 3 K=K1,K2,K3	001153
00525	140*	PA(K)=PA(K)+(1.-DEL(K))*DEL(K)	001153
00526	141*	CALL TEMP	001156
00527	142*	CALL TRANS	001160
00530	143*	RA(I)=CRL(I)	001162
00531	144*	TAUA=CTAUL(I)	001164
00532	145*	PA(K)=PA(K)+(1.-DEL(K))/(1.-DEL(K))	001166
00533	146*	CALL TEMP	001175
00534	147*	CALL TRANS	001177
00535	148*	RB(I)=CRL(I)	001201
00536	149*	TAUB=CTAUL(I)	001203
00537	150*	PA(K)=PA(K)/(1.-DEL(K))	001205
00540	151*	S(I,4)=(RA(I)-RB(I))/(DEL(K)*MRL(I)*2.)	001212
00541	152*	B(I,2,K)=(TAUB-TAUA)/(DEL(K)*(1.-MTAUL(I))*2.)	001220
00542	153*	3 CONTINUE	001227
00544	154*	CALL TEMP	001227
00545	155*	CALL TRANS	001231
00545	156*	C CHANGE DERIVATIVE VARIABLES TO CONDENSE ARRAY K=K1,K2,K3 TO K=1,KV	001231
00546	157*	4V=0	001233
00547	158*	DO 7 K=K1,K2,K3	001240

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## APPENDIX III

### EXAMPLE OF PROFILE PROGRAM DATA CARDS AND OUTPUT IN MODE = 1

Data Cards With Data For Five Wave Numbers (11 = 0).

Profile PROP = 2, Gases H<sub>2</sub>O and N<sub>2</sub>

04W4 402E1,PROFE,INAD1,PAWE100,115,NAVE1500,1100,5000,  
0130,3333,303,  
KRWV1,KNW45,7M1700,7C2033,7H2,50,7M450,7051:  
UPL1M1,3000,1,1,3000,00717M402,000,002,001,7113172,PR:  
PC1,05,002,7M1,05,000,7M1,05,000,7M1,05,000,7M1,05,000,7M1,05,000,  
1500,2000,2500,3000,3500,4000,4500,5000,5500,6000,  
3000,4000,5000,6000,7000,8000,9000,1000,1100,1200,1300,1400,1500,  
1600,1700,1800,1900,2000,2100,2200,2300,2400,2500,2600,2700,2800,2900,3000,3100,3200,3300,3400,3500,3600,3700,3800,3900,4000,4100,4200,4300,4400,4500,4600,4700,4800,4900,5000,5100,5200,5300,5400,5500,5600,5700,5800,5900,6000,6100,6200,6300,6400,6500,6600,6700,6800,6900,7000,7100,7200,7300,7400,7500,7600,7700,7800,7900,8000,8100,8200,8300,8400,8500,8600,8700,8800,8900,9000,9100,9200,9300,9400,9500,9600,9700,9800,9900,1000,1010,1020,1030,1040,1050,1060,1070,1080,1090,1100,1110,1120,1130,1140,1150,1160,1170,1180,1190,1200,1210,1220,1230,1240,1250,1260,1270,1280,1290,1300,1310,1320,1330,1340,1350,1360,1370,1380,1390,1400,1410,1420,1430,1440,1450,1460,1470,1480,1490,1500,1510,1520,1530,1540,1550,1560,1570,1580,1590,1600,1610,1620,1630,1640,1650,1660,1670,1680,1690,1700,1710,1720,1730,1740,1750,1760,1770,1780,1790,1800,1810,1820,1830,1840,1850,1860,1870,1880,1890,1900,1910,1920,1930,1940,1950,1960,1970,1980,1990,2000,2010,2020,2030,2040,2050,2060,2070,2080,2090,2100,2110,2120,2130,2140,2150,2160,2170,2180,2190,2200,2210,2220,2230,2240,2250,2260,2270,2280,2290,2300,2310,2320,2330,2340,2350,2360,2370,2380,2390,2400,2410,2420,2430,2440,2450,2460,2470,2480,2490,2500,2510,2520,2530,2540,2550,2560,2570,2580,2590,2600,2610,2620,2630,2640,2650,2660,2670,2680,2690,2700,2710,2720,2730,2740,2750,2760,2770,2780,2790,2800,2810,2820,2830,2840,2850,2860,2870,2880,2890,2900,2910,2920,2930,2940,2950,2960,2970,2980,2990,3000,3010,3020,3030,3040,3050,3060,3070,3080,3090,3100,3110,3120,3130,3140,3150,3160,3170,3180,3190,3200,3210,3220,3230,3240,3250,3260,3270,3280,3290,3300,3310,3320,3330,3340,3350,3360,3370,3380,3390,3400,3410,3420,3430,3440,3450,3460,3470,3480,3490,3500,3510,3520,3530,3540,3550,3560,3570,3580,3590,3600,3610,3620,3630,3640,3650,3660,3670,3680,3690,3700,3710,3720,3730,3740,3750,3760,3770,3780,3790,3800,3810,3820,3830,3840,3850,3860,3870,3880,3890,3900,3910,3920,3930,3940,3950,3960,3970,3980,3990,4000,4010,4020,4030,4040,4050,4060,4070,4080,4090,4100,4110,4120,4130,4140,4150,4160,4170,4180,4190,4200,4210,4220,4230,4240,4250,4260,4270,4280,4290,4300,4310,4320,4330,4340,4350,4360,4370,4380,4390,4400,4410,4420,4430,4440,4450,4460,4470,4480,4490,4500,4510,4520,4530,4540,4550,4560,4570,4580,4590,4600,4610,4620,4630,4640,4650,4660,4670,4680,4690,4700,4710,4720,4730,4740,4750,4760,4770,4780,4790,4800,4810,4820,4830,4840,4850,4860,4870,4880,4890,4900,4910,4920,4930,4940,4950,4960,4970,4980,4990,5000,5010,5020,5030,5040,5050,5060,5070,5080,5090,5100,5110,5120,5130,5140,5150,5160,5170,5180,5190,5200,5210,5220,5230,5240,5250,5260,5270,5280,5290,5300,5310,5320,5330,5340,5350,5360,5370,5380,5390,5400,5410,5420,5430,5440,5450,5460,5470,5480,5490,5500,5510,5520,5530,5540,5550,5560,5570,5580,5590,5600,5610,5620,5630,5640,5650,5660,5670,5680,5690,5700,5710,5720,5730,5740,5750,5760,5770,5780,5790,5800,5810,5820,5830,5840,5850,5860,5870,5880,5890,5900,5910,5920,5930,5940,5950,5960,5970,5980,5990,6000,6010,6020,6030,6040,6050,6060,6070,6080,6090,6100,6110,6120,6130,6140,6150,6160,6170,6180,6190,6200,6210,6220,6230,6240,6250,6260,6270,6280,6290,6300,6310,6320,6330,6340,6350,6360,6370,6380,6390,6400,6410,6420,6430,6440,6450,6460,6470,6480,6490,6500,6510,6520,6530,6540,6550,6560,6570,6580,6590,6600,6610,6620,6630,6640,6650,6660,6670,6680,6690,6700,6710,6720,6730,6740,6750,6760,6770,6780,6790,6800,6810,6820,6830,6840,6850,6860,6870,6880,6890,6900,6910,6920,6930,6940,6950,6960,6970,6980,6990,7000,7010,7020,7030,7040,7050,7060,7070,7080,7090,7100,7110,7120,7130,7140,7150,7160,7170,7180,7190,7200,7210,7220,7230,7240,7250,7260,7270,7280,7290,7300,7310,7320,7330,7340,7350,7360,7370,7380,7390,7400,7410,7420,7430,7440,7450,7460,7470,7480,7490,7500,7510,7520,7530,7540,7550,7560,7570,7580,7590,7600,7610,7620,7630,7640,76

[illegible]

## Printout of Input Data

[illegible]

**SEND**

GAS=	N20	N2						
ALPH=	1.00	.20	.00	.33	.33	.33	.27	.30
MTAB=	.2500	.4300	.3930	.3150	.2900	.2650	.0000	.0200
	.0040	.0117	.0372	.0804	.1383	.2199	.3273	.4333
	.3540	.2140	.0390	.0320	.0370	.0300	.0000	.0000
	.3066	.0211	.0395	.0503	.0610	.0710	.0000	.0000
	.3333	.0370	.0203	.0660	.0782	.0885	.0000	.0000
BTAB=	.107	.115	.309	.690	1.360	2.890	.000	.330
	.096	.113	.350	.553	2.450	18.000	.000	.300
	.144	.182	.320	.586	1.253	5.000	.000	.300
	.113	.157	.385	.780	1.450	5.210	.000	.300
	.075	.094	.187	.480	2.370	16.300	.000	.300



## Profiles and Computation

PROFILE PARAMETERS	TEMP EXPONENT N <sub>2</sub>	AXIAL TEMP T <sub>C,H</sub>	AXIAL PRESS P <sub>C,ATM</sub>	WALL TEMP T <sub>W,H</sub>	WALL PRESS P <sub>W,ATM</sub>	PRESS EXPONENT N <sub>2</sub>	
	.50030	2000.00	.35000	1700.00	.30000	.50000	
PARAMETER ERROR PERCENT	.08	-1.48	.68	4.58	WAVENUMBER(1/CM)	RESIDUAL,PERCENT	
	.0	3.6	-1.1	-6.9	3500.	2.08	
	.3	-0.0	7.0	.2	3100.	3.2	
	.3	.3	.3	.0	3500.	4.4	
	.0	.0	.0	.0	0.	.0	
RMS TOTAL	.0	4.0	7.1	8.2	0.	.0	
PARAMETER ENRO PERCENT	.08	-9.72	2.98	19.48	WAVENUMBER(1/CM)	RESIDUAL,PERCENT	
	.0	10.7	-3.1	-19.4	3500.	2.08	
	.3	.0	7.0	.0	3400.	7.3	
	.3	.3	.0	.0	3500.	4.4	
	.0	.0	.0	.0	0.	.0	
RMS TOTAL	.3	14.4	8.2	27.4	0.	.0	
PARAMETER ERROR PERCENT	.08	-2.28	.88	5.98	WAVENUMBER(1/CM)	RESIDUAL,PERCENT	
	.3	4.6	-1.3	-6.4	3500.	2.08	
	.0	-0.1	7.0	.3	4100.	3.6	
	.3	.3	.2	.0	3500.	4.4	
	.0	.0	.0	.0	0.	.0	
RMS TOTAL	.3	5.2	7.2	12.3	0.	.0	
PARAMETER ERROR PERCENT	.08	-1.48	.58	4.48	WAVENUMBER(1/CM)	RESIDUAL,PERCENT	
	.0	4.8	-1.4	-8.6	3500.	2.08	
	.3	-0.1	7.0	.2	3000.	4.3	
	.3	.3	.0	.0	3500.	4.4	
	.0	.0	.0	.0	0.	.0	
RMS TOTAL	.3	4.9	7.2	9.7	0.	.0	
WAVENUMBER(1/CM):	3500.	3100.	3400.	4100.	3300.	0.	
TRANSMITTANCE:	.598	.822	.602	.854	.885	.000	
TEMPERATURE PROFILE	PARTIAL PRESSURE PROFILES EACH GAS,ATM						
X,CM	TEMP,H	420	N <sub>2</sub>				
.00	1700.00	.3300	.6900	.0000	.0000	.0000	.0000
.50	1705.97	.3313	.6990	.0000	.0000	.0000	.0000
1.00	1711.88	.3320	.6980	.0000	.0000	.0000	.0000
2.50	1729.25	.3349	.6951	.0000	.0000	.0000	.0000
5.00	1757.30	.3395	.6905	.0000	.0000	.0000	.0000
13.33	1838.33	.3183	.6820	.0000	.0000	.0000	.0000
15.00	1853.30	.3255	.6745	.0000	.0000	.0000	.0000
23.33	1892.33	.3323	.6680	.0000	.0000	.0000	.0000
25.33	1925.00	.3375	.6625	.0000	.0000	.0000	.0000
35.00	1973.30	.3455	.6545	.0000	.0000	.0000	.0000
50.00	2000.00	.3503	.6500	.0000	.0000	.0000	.0000
65.33	1973.33	.3455	.6545	.0000	.0000	.0000	.0000
75.00	1925.30	.3375	.6625	.0000	.0000	.0000	.0000
83.33	1892.33	.3323	.6680	.0000	.0000	.0000	.0000
85.00	1853.30	.3255	.6745	.0000	.0000	.0000	.0000
93.00	1808.00	.3183	.6820	.0000	.0000	.0000	.0000
95.00	1757.30	.3395	.6905	.0000	.0000	.0000	.0000
97.50	1729.25	.3349	.6951	.0000	.0000	.0000	.0000
99.00	1711.88	.3323	.6980	.0000	.0000	.0000	.0000
99.50	1735.97	.3313	.6990	.0000	.0000	.0000	.0000
100.33	1733.33	.3300	.7000	.0000	.0000	.0000	.0000

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## APPENDIX I

## EXAMPLE OF PROFILE PROGRAM DATA CARDS AND OUTPUT IN MODE - 3

Data Cards Continued From Cards of APPENDIX H, With Data For

Four Wave Numbers (11-4), Profile PROF = 3

\$NAME MODE=3,11=4 \$  
 \$NAME PW=.36,.64,4\*0. \$

## Printout of Input Data

```

NAME =
MODE = 03
PROF = 02
IREAD = 03
PATH = .10000000E+33
I1 = 04
WAVE = .35333000E+34, .31030000E+34, .34333333E+34, .41000000E+04,
      .30003000E+34, .00000000E+00, .00033033E+30, .00000000E+00
HRL = .37609724E-32, .37728009E-02, .37566974E-02, .38719275E-02,
      .37332037E-32, .00030000E+33, .03333333E+30, .33303330E+00
MTAUL = .59631328E+00, .82238571E+00, .60239885E+00, .85361033E+00,
      .88483335E+33, .03030000E+00, .00000030E+00, .00000000E+00
ERRV = .10003000E+31
ERRK = .50003000E+01
TM = .17333000E+34
TC = .20003000E+34
NT = .50003000E+00
TWD = .33333000E+33
JB = 01
UPLIM = .10003000E+01, .30000000E+04, .10330030E+01, .30000000E+04
BOTLIM = .23333000E-31, .60000000E+33, .23333330E-31, .60303330E+03
L1 = 01
L2 = 02
PS = .13333000E+31
PC = .35003000E+30, .65000000E+00, .00333030E+30, .00003330E+00,
      .00003000E+30, .00000000E+00, .50003030E+33, .33303330E+00
NP = .53333000E+33, .50003030E+33, .03333330E+30, .33303330E+00,
      .30003000E+30, .00000000E+00
PW = .30003000E+30, .70000000E+00, .00000030E+30, .00000000E+00,
      .30003000E+30, .03030000E+33
NK = 06
TKTAR = .60003000E+33, .10000000E+04, .15033030E+04, .20000000E+04,
      .25333000E+34, .33030000E+34, .03333330E+30, .33303330E+03
NB = 06
TBTAR = .60003000E+33, .10000000E+04, .15000030E+34, .20000000E+04,
      .25033000E+34, .30000000E+34, .03333330E+30, .33303330E+03
J1 = 21
Z = .33333000E+33, .13030030E-31, .23333330E-01, .50000000E-01,
      .10003000E+30, .20000000E+00, .30030030E+30, .40000000E+00,
      .50003000E+30, .70000000E+00, .10030030E+01, .10000000E+01,
      .10333000E+31, .10030000E+31, .13333330E+31, .10000000E+01,
      .10003000E+01, .10000000E+01, .10030030E+01, .10000000E+01,
      .13333000E+31
ITER = 10
TX = .30003000E+00
SEND

```

SNAM1	:				
MODE	:		+2		
PROF	:		+2		
IRFAN	:		+3		
PATM	:	.10000000E+03			
II	:		+4		
HAVE	:	.35000000E+04,	.31000000E+04,	.34000000E+04,	.41000000E+04,
		.30000000E+04,	.00000000E+00,	.00000000E+00,	.00000000E+00,
HRL	:	.37500000E+02,	.37700000E+02,	.37500000E+02,	.36700000E+02,
		.37500000E+02,	.00000000E+00,	.00000000E+00,	.00000000E+00,
HTAUL	:	.59400000E+00,	.02200000E+00,	.00200000E+00,	.05300000E+00,
		.00400000E+00,	.00000000E+00,	.00000000E+00,	.00000000E+00,
ERRV	:	.10000000E+01			
ERRA	:	.50000000E+01			
TM	:	.17000000E+04			
TC	:	.20000000E+04			
NT	:	.50000000E+03			
TWD	:	.00000000E+00			
JB	:	+1			
UPLIM	:	.10000000E+01,	.30000000E+04,	.10000000E+01,	.30000000E+04,
BOTLIM	:	.20000000E+01,	.60000000E+03,	.20000000E+01,	.60000000E+03,
L1	:	+1			
L2	:	+2			
PS	:	.10000000E+01			
PC	:	.35000000E+00,	.60000000E+00,	.00000000E+00,	.00000000E+00,
		.30000000E+00,	.70000000E+00,	.00000000E+00,	.00000000E+00,
NP	:	.50000000E+00,	.50000000E+00,	.00000000E+00,	.00000000E+00,
		.00000000E+00,	.00000000E+00,	.00000000E+00,	.00000000E+00,
PM	:	.36000000E+00,	.60000000E+00,	.00000000E+00,	.00000000E+00,
		.00000000E+00,	.00000000E+00,	.00000000E+00,	.00000000E+00,
NK	:	+6			
HTAUL	:	.60000000E+03,	.10000000E+04,	.15000000E+04,	.20000000E+04,
		.25000000E+04,	.00000000E+04,	.00000000E+04,	.00000000E+04,
NB	:	+6			
HTAUL	:	.60000000E+03,	.10000000E+04,	.15000000E+04,	.20000000E+04,
		.25000000E+04,	.00000000E+04,	.00000000E+04,	.00000000E+04,
J1	:	+21			
Z	:	.00000000E+00,	.10000000E+01,	.20000000E+01,	.50000000E+01,
		.10000000E+00,	.20000000E+00,	.30000000E+00,	.40000000E+00,
		.50000000E+00,	.70000000E+00,	.10000000E+01,	.10000000E+01,
		.10000000E+01,	.10000000E+01,	.10000000E+01,	.10000000E+01,
		.10000000E+01,	.10000000E+01,	.10000000E+01,	.10000000E+01,
ITER	:	+10			
TX	:	.00000000E+00			
SEND	:				

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## Computation and Profiles

PROFIL PARAMETERS	TEMP EXONENT NY	AXIAL TEMP TC,K	AXIAL PRESS PC,ATM	WALL TEMP TW,K	WALL PRESS PW,ATM	PYFCS EXONENT NP			
	.51000	2000.00	.35000	1733.00	.35000	.50000			
INCREMENTS DPA	.00000	.00	.00000	.00	ITERATION= 1	RMS RESIDUAL=	.399-01	STEP=	.000
PARAMETERS PA	.50000	2000.00	.35000	1700.00	RESIDUALS=	-.111-01	-.747-02	-.105-01	-.892-02
				WAVENUMBER(1/CM)=		3500.	3100.	3400.	4100.
INCREMENTS DPA	.00000	3.10	-.01824	10.42	ITERATION= 1	RMS RESIDUAL=	.160-02	STEP=	.129-01
PARAMETERS PA	.50000	2020.12	.33176	1717.42	RESIDUALS=	-.629-03	.442-04	-.631-03	.620-03
				WAVENUMBER(1/CM)=		3500.	3100.	3400.	4100.
INCREMENTS DPA	.00000	-1.51	-.00053	1.49	ITERATION= 2	RMS RESIDUAL=	.626-03	STEP=	.311-02
PARAMETERS PA	.50000	2031.29	.33122	1713.91	RESIDUALS=	-.410-05	-.372-03	-.228-03	.445-03
				WAVENUMBER(1/CM)=		3500.	3100.	3400.	4100.
INCREMENTS DPA	.00000	-.05	.00000	.13	ITERATION= 3	RMS RESIDUAL=	.623-03	STEP=	.113-03
PARAMETERS PA	.50000	2031.23	.33126	1714.03	RESIDUALS=	.260-04	-.375-03	-.204-03	.453-03
				WAVENUMBER(1/CM)=		3500.	3100.	3400.	4100.
INCREMENTS DPA	.00000	.00	.00000	.00	ITERATION= 4	RMS RESIDUAL=	.623-03	STEP=	.929-06
PARAMETERS PA	.50000	2031.23	.33126	1714.04	RESIDUALS=	.207-04	-.375-03	-.203-03	.453-03
				WAVENUMBER(1/CM)=		3500.	3100.	3400.	4100.
PARAMETER ERROR PERCENT	.08	-1.37	.48	3.28	WAVENUMBER(1/CM)	RESIDUAL PERCENT			
	.0	2.0	-.7	-4.5	3500.	7.08			
	.0	-.7	.2	1.9	3100.	3.2			
	.0	1.4	-.4	-1.0	3400.	2.0			
	.0	-.1	7.1	.2	4100.	3.6			
RMS TOTAL	.0	3.5	7.1	6.6	3500.	4.4			
					0.	.0			
WAVENUMBER(1/CM)=	3500.	3100.	3400.	4100.	3500.	3100.	3400.	4100.	3500.
TRANSMITTANCE=	.598	.822	.602	.853	.030	.000	.000	.000	.000
TEMPERATURE PROFILE	PARTIAL PRESSURE PROFILES EACH GAS,ATM								
X,CM	TEMP,K	420	N2						
.00	1714.34	.3437	.6593	.0000	.0000	.0000	.0000	.0000	
.50	1719.75	.3405	.6595	.0000	.0000	.0000	.0000	.0000	
1.00	1725.41	.3403	.6597	.0000	.0000	.0000	.0000	.0000	
2.50	1742.34	.3398	.6602	.0000	.0000	.0000	.0000	.0000	
5.00	1766.60	.3389	.6611	.0000	.0000	.0000	.0000	.0000	
10.00	1817.43	.3373	.6627	.0000	.0000	.0000	.0000	.0000	
15.00	1862.51	.3359	.6641	.0000	.0000	.0000	.0000	.0000	
20.00	1897.84	.3347	.6653	.0000	.0000	.0000	.0000	.0000	
25.00	1929.43	.3336	.6664	.0000	.0000	.0000	.0000	.0000	
35.00	1975.38	.3321	.6679	.0000	.0000	.0000	.0000	.0000	
50.00	2001.23	.3313	.6687	.0000	.0000	.0000	.0000	.0000	
65.00	1975.38	.3321	.6679	.0000	.0000	.0000	.0000	.0000	
75.00	1929.43	.3336	.6664	.0000	.0000	.0000	.0000	.0000	
80.00	1897.84	.3347	.6653	.0000	.0000	.0000	.0000	.0000	
85.00	1860.51	.3359	.6641	.0000	.0000	.0000	.0000	.0000	
90.00	1817.43	.3373	.6627	.0000	.0000	.0000	.0000	.0000	
95.00	1766.60	.3389	.6611	.0000	.0000	.0000	.0000	.0000	
97.50	1742.34	.3398	.6602	.0000	.0000	.0000	.0000	.0000	
99.00	1725.41	.3403	.6597	.0000	.0000	.0000	.0000	.0000	
99.50	1719.75	.3405	.6595	.0000	.0000	.0000	.0000	.0000	
100.00	1714.34	.3437	.6593	.0000	.0000	.0000	.0000	.0000	

## APPENDIX J

EXAMPLE OF WAVES PROGRAM DATA CARDS AND OUTPUT  
Data Cards With Data For Four Wave Numbers (I1 = 4), Gases H<sub>2</sub>O and N<sub>2</sub>

```

$NAME1 PROF=1, IREAD=1, PATH=170, I1=4, WAVE=3100, 3500, 3775, 4100, 4400,
      JR=1, UPLIM=1, 3500, 2, 3000, 25, 70, 20, 02,
      L1=1, L2=2, PS=1, PC=15, 65, 400, NP=5, 5, 400, PN=3, 70, 400,
      NK=6, TAYAR=633, 1033, 1533,
      2000, 2500, 3000, 3500, 4000, 4500, 5000, 5500, 6000, 6500, 7000, 7500, 8000,
      30, 70, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800,
      N20 N2
      1. 2
      .0048 .0137 .0372 .0864 .133 .129
      .250 .430 .393 .315 .208 .265
      .174 .120 .110 .115 .115 .109
      .0086 .0211 .0395 .0503 .0610 .0710
      .094 .113 .145 .236 .550 2.450
      .107 .145 .309 .690 1.360 14.000
      .233 .264 .374 .653 1.413 2.893
      .113 .157 .345 .780 1.850 5.210

```

## Printout of Input Data

```

$NAME1
IREAD = 1
PROF = 1
PATH = 170
I1 = 4
WAVE = 3100, 3500, 3775, 4100, 4400
TN = 1
TC = 2
NT = 25
TWR = 70
JB = 20
UPLIM = 1
BOTLIM = 2
L1 = 1
L2 = 2
PS = 15
PC = 65
NP = 400
PN = 5
NK = 6
TAYAR = 633, 1033, 1533, 2000, 2500, 3000, 3500, 4000, 4500, 5000, 5500, 6000, 6500, 7000, 7500, 8000
NR = 30
TBTAR = 70, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800
K4 = 100
NPA = 150
PA1 = 200
J1 = 250
Z = 300
ITER = 10
SEND
GAS= H2O N2
ALPH2 1.00 .20 .00 .00 .00 .00 .00 .00
KTAB= .0048 .0137 .0372 .0864 .133 .129 .250 .430 .393 .315 .208 .265 .174 .120 .110 .115 .115 .109 .0086 .0211 .0395 .0503 .0610 .0710 .094 .113 .145 .236 .550 2.450 .107 .145 .309 .690 1.360 14.000 .233 .264 .374 .653 1.413 2.893 .113 .157 .345 .780 1.850 5.210
BTAB= .0048 .0137 .0372 .0864 .133 .129 .250 .430 .393 .315 .208 .265 .174 .120 .110 .115 .115 .109 .0086 .0211 .0395 .0503 .0610 .0710 .094 .113 .145 .236 .550 2.450 .107 .145 .309 .690 1.360 14.000 .233 .264 .374 .653 1.413 2.893 .113 .157 .345 .780 1.850 5.210

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## Profiles and Computation

TEMPERATURE PROFILE		PARTIAL PRESSURE PROFILES EACH GAS, ATM					
X, CM	TEMP, °	H <sub>2</sub> O	N <sub>2</sub>				
.00	1330.00	.3300	.7000	.0000	.0000	.0000	.0000
.50	1339.40	.3313	.6990	.0000	.0000	.0000	.0000
1.00	1077.63	.3323	.6980	.0000	.0000	.0000	.0000
2.50	1125.49	.3349	.6951	.0000	.0000	.0000	.0000
5.00	1343.90	.3395	.6935	.0000	.0000	.0000	.0000
10.00	1590.40	.3180	.6920	.0000	.0000	.0000	.0000
15.00	1759.90	.3255	.6745	.0000	.0000	.0000	.0000
20.00	1870.40	.3323	.6680	.0000	.0000	.0000	.0000
25.00	1937.50	.3375	.6625	.0000	.0000	.0000	.0000
35.00	1991.90	.3455	.6545	.0000	.0000	.0000	.0000
50.00	2200.00	.3500	.6500	.0000	.0000	.0000	.0000
65.00	1991.90	.3455	.6545	.0000	.0000	.0000	.0000
75.00	1937.50	.3375	.6625	.0000	.0000	.0000	.0000
80.00	1870.40	.3323	.6680	.0000	.0000	.0000	.0000
85.00	1759.90	.3255	.6745	.0000	.0000	.0000	.0000
90.00	1590.40	.3180	.6920	.0000	.0000	.0000	.0000
95.00	1343.90	.3395	.6905	.0000	.0000	.0000	.0000
97.50	1125.49	.3349	.6951	.0000	.0000	.0000	.0000
99.00	1077.63	.3323	.6980	.0000	.0000	.0000	.0000
99.50	1039.40	.3313	.6990	.0000	.0000	.0000	.0000
100.00	1000.00	.3300	.7000	.0000	.0000	.0000	.0000

PROFILE PARAMETERS	TEMP EXPONENT NT	AXIAL TEMP TC, K	AXIAL PRESS PC, ATM	WALL TEMP TW, K	WAVELENGTH (1/CM)	LAST ITERATION	RMS RESIDUAL
PARAMETERS PA	.05000	1934.37	.33712	1000.00	3100.	3	.996-37
PARAMETERS PA	.13000	1928.85	.34025	1000.00	3100.	2	.126-06
PARAMETERS PA	.15000	1931.90	.34395	1000.00	3100.	2	.894-07
PARAMETERS PA	.20000	1976.28	.34659	1000.00	3100.	2	.996-07
PARAMETERS PA	.33000	2021.18	.35001	1000.00	3100.	3	.332-34
PARAMETERS PA	.40000	2063.31	.34800	1000.00	3100.	3	.225-35
PARAMETERS PA	.50000	2135.49	.34832	1000.00	3100.	2	.767-04

PARAMETERS PA	.63300	2144.81	.34936	1000.00	3170.	2	.437-04
PARAMETERS PA	.05000	1834.74	.36788	1000.00	3530.	3	.722-05
PARAMETERS PA	.10000	1884.00	.36068	1033.30	3500.	2	.138-35
PARAMETERS PA	.15000	1925.00	.35466	1000.00	3500.	2	.251-36
PARAMETERS PA	.20000	1963.77	.35223	1333.30	3530.	2	.144-06
PARAMETERS PA	.30000	2031.58	.34620	1000.00	3500.	2	.545-04
PARAMETERS PA	.40000	2091.55	.34035	1000.00	3500.	2	.722-05
PARAMETERS PA	.50000	2150.02	.33668	1033.30	3500.	2	.617-35
PARAMETERS PA	.60000	2205.47	.33533	1000.00	3530.	2	.287-05
PARAMETERS PA	.35000	1839.94	.35545	1333.30	3775.	3	.271-04
PARAMETERS PA	.13000	1883.20	.35384	1000.00	3775.	2	.230-06
PARAMETERS PA	.15000	1923.17	.35244	1000.00	3775.	2	.634-07
PARAMETERS PA	.20000	1962.10	.35107	1033.30	3775.	2	.684-37
PARAMETERS PA	.30000	2034.16	.34650	1000.00	3775.	2	.117-34
PARAMETERS PA	.40000	2099.36	.34027	1333.30	3775.	2	.653-05
PARAMETERS PA	.50000	2162.49	.33581	1000.00	3775.	2	.278-05
PARAMETERS PA	.60000	2222.74	.33276	1000.00	3775.	2	.741-06
PARAMETERS PA	.05000	1882.26	.34533	1033.30	4100.	3	.173-34
PARAMETERS PA	.13000	1912.02	.34667	1000.00	4130.	2	.689-37
PARAMETERS PA	.15000	1941.17	.34788	1333.30	4130.	2	.114-06
PARAMETERS PA	.23000	1973.48	.34898	1333.30	4130.	2	.544-07
PARAMETERS PA	.30000	2028.86	.34942	1000.00	4100.	2	.508-04
PARAMETERS PA	.40000	2086.02	.34815	1000.00	4100.	2	.966-06
PARAMETERS PA	.50000	2142.23	.34760	1333.30	4130.	2	.648-36
PARAMETERS PA	.60000	2196.28	.34756	1000.00	4130.	2	.420-06

DEPENDENT PARAMETER TC,M WITH ZETA= -.57+03

NY WAVENUMBER (1/CN)	.050	.100	.150	.200	.300	.400	.500	.600	.600	.600
3100.	2018.593	2014.517	2009.089	2004.835	1992.628	1977.652	1962.721	1944.929	.000	.000
3500.	1949.232	1969.663	1982.106	1992.329	2033.023	2035.885	2037.253	2005.589	.000	.000
3775.	1954.161	1968.863	1980.276	1990.654	2005.611	2013.694	2019.719	2022.863	.000	.000
4100.	1996.476	1997.681	1998.276	1999.134	2003.308	2003.361	1999.428	1996.399	.000	.000

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## APPENDIX K

### EXAMPLE OF PROFILE WITH HIGH-TEMPERATURE CORE

Data Cards With Measured Data, Two Wave Numbers, Profile PROF = 2

### No Boundary Layer, Gases H<sub>2</sub>O and N<sub>2</sub>

```

NAME=2,PROF=2,IREAD=1,PATH=100,11=2,WAVE=3537,3100,603,
WFL=3,37113,003433,603,MTAUL=4316,6352,607,
EPRV=1,EPRK=5,TW=1,03,TC=1859,NT=53,T8=1130,J6=5,UPLTW=1,3530,
1,3000,90TLIN=.02,603,02,50R,LL1=1,LL2=2,PS=1,PC=35,65,403,
NP=25,5,03,PM=3,7,403,NK=6,TXAH=673,1333,1533,2030,2530,
3330,2*0,N8=6,TSTAT=503,1000,1500,2000,2500,7303,2*0,
1,1=25,Z=3,03,02,045,1,2,3,4,5,6,7,8,901,
ITLR=10,TK=C03. 4
W20 N2
1. .2
.258 .438 .393 .315 .248 .265
.0644 .0137 .0372 .0864 .133 .129
.326 .525 1.13 2.13 3.35 4.35
.94 .113 .236 .553 2.45 18.0

```

### Printout of Input Data

NAME1	=			
MODL	=	+2		
PROF	=	+2		
IREAD	=	+1		
PATH	=	.10000000E+00		
II	=	+2		
WAVE	=	.35000000E+00	.31000000E+00	.00000000E+00
MRL	=	.31130000E+00	.34330000E+00	.00000000E+00
HTAUL	=	.43160000E+00	.33520000E+00	.00000000E+00
ERRV	=	.10000000E+00	.00000000E+00	.00000000E+00
LRRN	=	.50000000E+00		
TW	=	.12000000E+00		
TC	=	.18500000E+00		
NT	=	.50000000E+00		
TWR	=	.11000000E+00		
JB	=	+5		
UPLIM	=	.10000000E+00	.30000000E+00	.30000000E+00
BOPLIM	=	.20000000E+00	.60000000E+00	.60000000E+00
L1	=	+1		
L2	=	+2		
PS	=	.10000000E+00		
PC	=	.35000000E+00	.65000000E+00	.00000000E+00
NP	=	.50000000E+00	.50000000E+00	.00000000E+00
PW	=	.30000000E+00	.70000000E+00	.00000000E+00
NK	=	+6		
TKTAR	=	.60000000E+00	.10000000E+00	.15000000E+00
NB	=	+6		
TBTAR	=	.60000000E+00	.10000000E+00	.15000000E+00
J1	=	+25		
Z	=	.00000000E+00	.10000000E+00	.20000000E+00
ITER	=	+10		
TX	=	.30000000E+00		

SEND

GAS=	H2O	N2	CO2	CH4	HCN	CO	H2	NO
ALPH=	1.00	.20	.00	.00	.30	.00	.00	.30
KTAB=	.2583	.4390	.3930	.3150	.2480	.2653	.0000	.0000
	.0048	.0137	.0172	.0864	.1733	.1293	.3333	.0333
STAB=	.326	.525	1.100	2.180	3.353	4.353	.333	.333
	.094	.113	.236	.550	2.453	18.003	.300	.300



## Computation and Profiles

PROFILE PARAMETERS	TEMP EXPONENT NT	AXIAL TEMP TC,K	AXIAL PRESS PC,ATM	WALL TEMP TW,K	WALL PRESS PW,ATM	PRESS EXPONENT NP				
	.50000	1850.00	.35000	1200.00	.30000	.50000				
INCREMENTS CPA	.03000	.00	.00000	.00	ITERATION= 0	RMS RESIDUAL= .342+00	STEP= .003			
PARAMETERS PA	.53003	1850.00	.35000	1200.00	RESIDUALS=	-.274+00	-.204+00	.165-01	.000	.000
					WAVENUMBER(1/CM)=	3500.	3100.	3500.	0.	0.
INCREMENTS CPA	.33003	42.66	-.00057	120.00	ITERATION= 1	RMS RESIDUAL= .220+00	STEP= .123+00			
PARAMETERS PA	.63000	1892.66	.34943	1320.00	RESIDUALS=	-.176+00	-.132+00	.132-01	.000	.000
					WAVENUMBER(1/CM)=	3500.	3100.	3500.	0.	0.
INCREMENTS CPA	.03003	56.15	-.00019	132.00	ITERATION= 2	RMS RESIDUAL= .646-01	STEP= .130+00			
PARAMETERS PA	.83000	1948.81	.34925	1452.00	RESIDUALS=	-.513-01	-.392-01	.231-02	.000	.000
					WAVENUMBER(1/CM)=	3500.	3100.	3500.	0.	0.
INCREMENTS CPA	.33003	24.93	.00066	47.19	ITERATION= 3	RMS RESIDUAL= .982-03	STEP= .455-01			
PARAMETERS PA	.53000	1973.70	.34991	1499.19	RESIDUALS=	.747-03	.636-03	-.198-03	.000	.000
					WAVENUMBER(1/CM)=	3500.	3100.	3500.	0.	0.
INCREMENTS CPA	.33003	-.42	.00010	-.52	ITERATION= 4	RMS RESIDUAL= .992-07	STEP= .585-03			
PARAMETERS PA	.53000	1973.29	.35000	1498.67	RESIDUALS=	.596-07	.447-07	-.655-07	.000	.000
					WAVENUMBER(1/CM)=	3500.	3100.	3500.	0.	0.
PARAMETER ERROR PERCENT	.0%	-.7%	.2%	3.5%	WAVENUMBER(1/CM)	RESIDUAL PERCENT				
	.0	2.8	.0	-7.0	3500.	1.6%				
	.0	-.1	6.3	.6	3100.	3.3				
	.0	.3	.0	.0	3500.	3.4				
	.0	.0	.0	.0	0.	.0				
	.0	.0	.0	.0	0.	.0				
RMS TOTAL	.0	2.9	6.3	7.8	0.	.0				
WAVENUMBER(1/CM)=	3500.	3100.	.0	.0	.0	.0	.0	.0		
TRANSMITTANCE=	.432	.835	.000	.000	.000	.000	.000	.000		
TEMPERATURE PROFILE										
X,CM	TEMP,K									
.00	1100.00	.3303	.7000	.0000	.0000	.0300	.0000			
.50	1185.19	.3313	.6990	.0333	.0333	.0300	.3303			
1.00	1262.32	.3323	.6980	.0333	.0333	.0300	.0303			
2.50	1445.28	.3349	.6951	.0003	.0003	.0000	.0000			
5.33	1588.85	.3395	.6905	.0333	.0333	.0000	.0000			
10.00	1669.53	.3180	.6820	.0000	.0000	.0000	.0000			
15.00	1740.73	.3255	.6745	.0000	.0000	.0300	.0000			
20.00	1802.43	.3323	.6680	.0333	.0333	.0300	.3303			
25.00	1854.63	.3375	.6625	.0000	.0000	.0000	.0000			
30.00	1897.35	.3423	.6580	.0333	.0333	.0300	.3303			
35.00	1930.57	.3455	.6545	.0000	.0000	.0300	.0000			
40.00	1954.33	.3483	.6520	.0000	.0000	.0300	.0000			
50.00	1973.29	.3500	.6500	.0000	.0000	.0300	.0000			
60.00	1954.39	.3483	.6520	.0000	.0000	.0300	.0000			
65.00	1930.57	.3455	.6545	.0000	.0333	.0300	.3303			
70.00	1897.35	.3423	.6580	.0000	.0000	.0300	.0000			
75.00	1854.63	.3375	.6625	.0333	.0333	.0300	.3303			
80.00	1802.43	.3323	.6680	.0000	.0000	.0300	.0000			
85.00	1740.73	.3255	.6745	.0333	.0333	.0300	.3303			
90.00	1669.53	.3180	.6820	.0000	.0000	.0000	.0000			
95.00	1588.85	.3395	.6905	.0000	.0000	.0300	.0000			
97.50	1445.28	.3349	.6951	.0000	.0000	.0000	.0000			
99.00	1262.32	.3323	.6980	.0000	.0000	.0300	.0000			
99.50	1185.19	.3313	.6990	.0000	.0333	.0300	.3303			
100.00	1100.00	.3303	.7000	.0000	.0000	.0300	.0000			

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TABLE I. - COEFFICIENTS TO BE USED IN EQUATION (16)

$\beta/\beta_e$	$A_1$	$A_2$	$A_3$	$A_4$	$A_5$
0	-0.68	-0.35	0.55	0.07	1.00
2	-.37	.62	.71	.43	1.37
5	.60	3.15	.90	.79	1.93
10	3.19	9.25	1.15	1.30	2.85
20	9.10	22.3	1.63	2.26	4.70
50	29.1	67.1	2.78	4.56	10.25
100	105	209	4.05	7.09	19.50

TABLE II. - SPECTRAL LINE BROADENING COEFFICIENT,

 $\alpha^*$  (FROM REF. 16)

Absorbing gas	Broadening gas						
	H <sub>2</sub> O	CO <sub>2</sub>	CO	CH <sub>4</sub>	N <sub>2</sub>	H <sub>2</sub>	O <sub>2</sub>
H <sub>2</sub> O	1	0.77			0.20	0.1	
CO <sub>2</sub>		1			.77	1.17	0.81
CO			1	1.12	.95	.85	
CH <sub>4</sub>		1.25		1	.75		

TABLE III. - ESTIMATED PERCENT ERROR OF  $T_c$  AND  $T_w^*$ 

AND TRANSMITTANCE FOR VARIOUS PATH LENGTHS

FOR PROFILE OF FIGURE 1(b)

[Measurement wavenumbers 3100, 3400, 3500, and 4100  $\text{cm}^{-1}$ ;

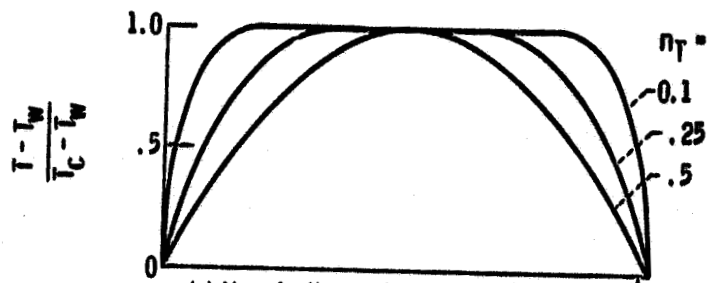
$T_c = 2000 \text{ K}$ ,  $n_T = 0.5$ ,  $p_c = 0.35 \text{ atm}$ ,  $p_w = 0.30 \text{ atm}$ ,  
 $n_p = 0.5$ . Errors caused by one percent error of radiance  
 measurement, and five percent error of tabulated absorp-  
 tion coefficients.]

Percent error in $T_c$				
$T_w^*$ , K	Path length, cm			
	50	100	200	400
1200	3.0	2.1	1.4	1.0
2000	11.5	6.3	4.2	3.2
Percent error in $T_w^*$				
1200	14.1	9.7	6.5	4.4
2000	20.0	9.8	5.7	3.8
Transmittance at 3500 $\text{cm}^{-1}$				
1200	0.703	0.591	0.465	0.333
2000	.713	.602	.476	.343

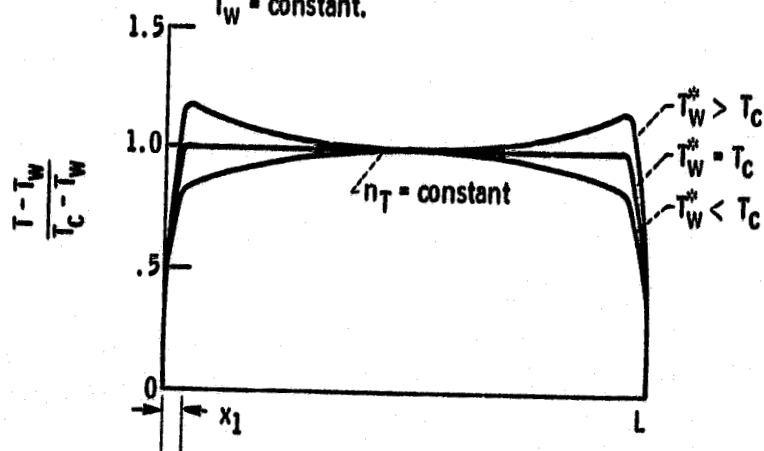
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TABLE IV. - PARAMETER INDEX CONTROL

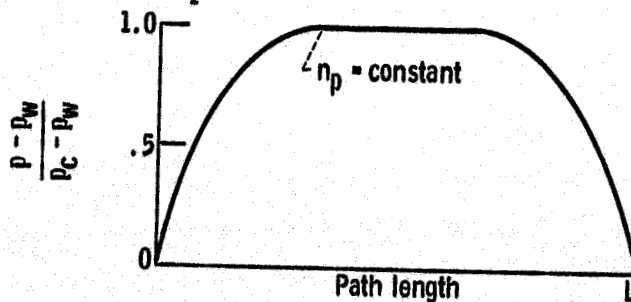
KEY	KEY1(KEY)	KEY2(KEY)	KEY3(KEY)	Variable parameters	
	K1	K2	K3	Fig. 1(a), PROF=1	Fig. 1(b), PROF=2
1	1	3	1	$n_T T_c p_c$	$T_c p_c T_w^*$
2	1	2	1	$n_T T_c$	$T_c p_c$
3	1	3	2	$n_T p_c$	$T_c T_w^*$
4	1	1	1	$n_T$	$T_c$
5	2	3	1	$T_c p_c$	$p_c T_w^*$
6	2	2	1	$T_c$	$p_c$
7	3	3	1	$p_c$	$T_w^*$
8	0	0	0	None	None



(a) Non-isothermal temperature profiles,  $T_W = \text{constant}$ .



(b) Near-isothermal temperature profiles, with  $T_W = \text{constant}$  and boundary layer thickness  $x_1 = \text{constant}$ .



(c) Partial pressure profile for each absorbing gas.

Figure 1. - Assumed profile functions.

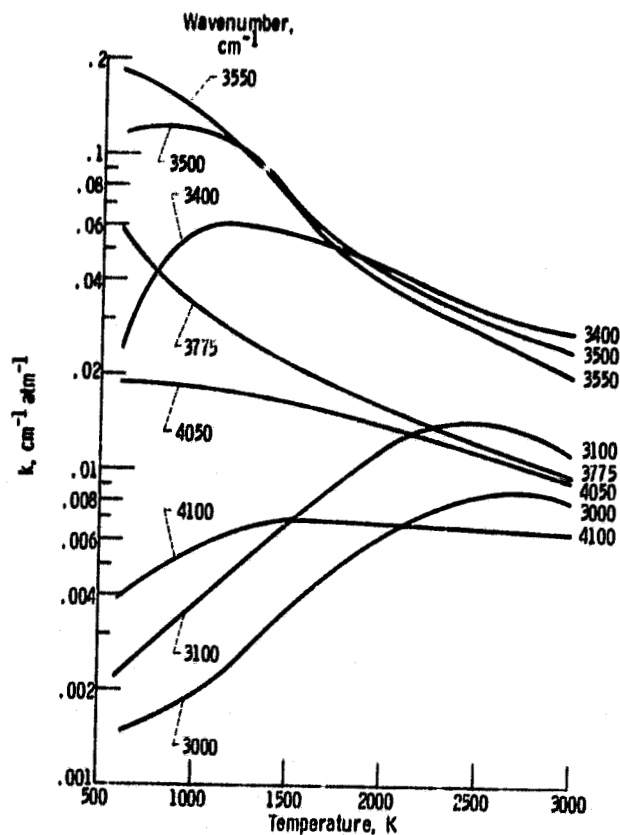


Figure 2. - Absorption coefficient for  $H_2O$ .

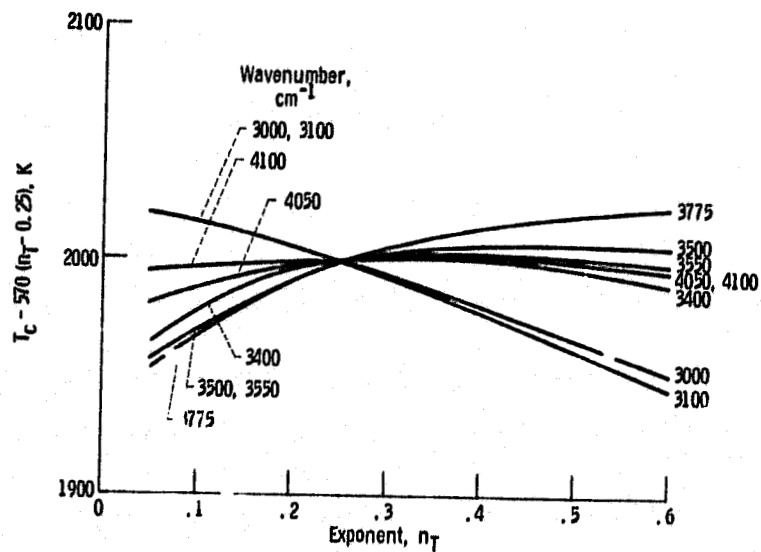


Figure 3. - Test of wavenumbers for profile of figure 1(a) with  $T_w = 1000$  K,  $p_c = 0.35$  atm,  $p_w = 0.30$  atm,  $n_D = 0.50$ , path length 100 cm Hydrogen-air combustion at 1 atm.



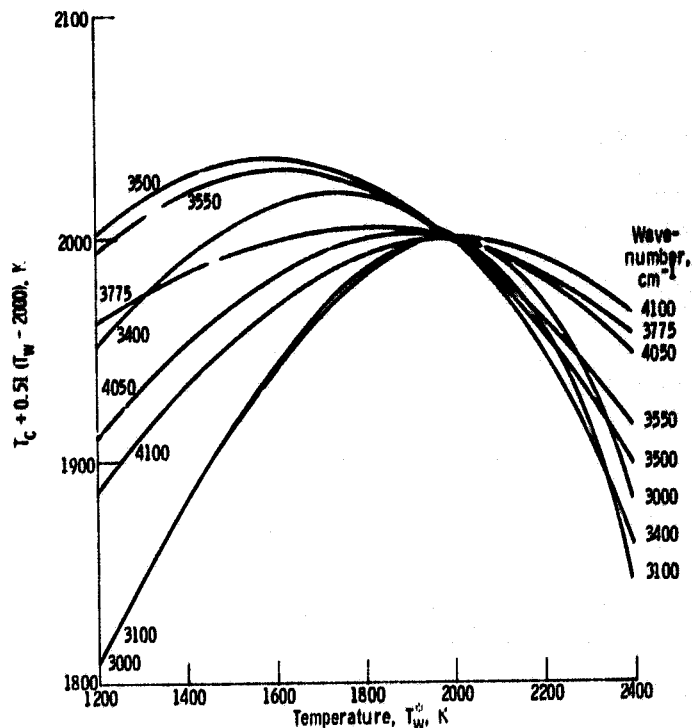


Figure 4. - Test of wavenumbers for profile of figure 1(b) with  $n_T = 0.5$ ,  $p_C = 0.35$  atm,  $p_W = 0.30$  atm,  $n_D = 0.50$ , path length 100 cm. Hydrogen-air combustion at 1 atm.

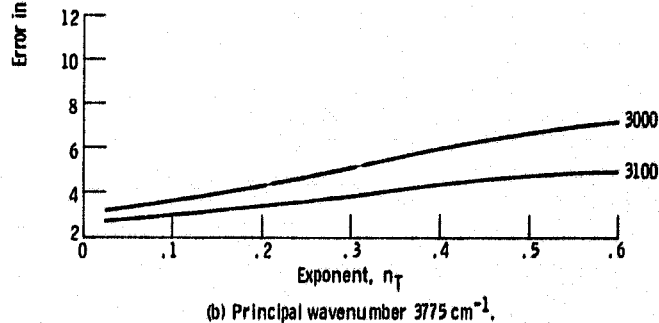
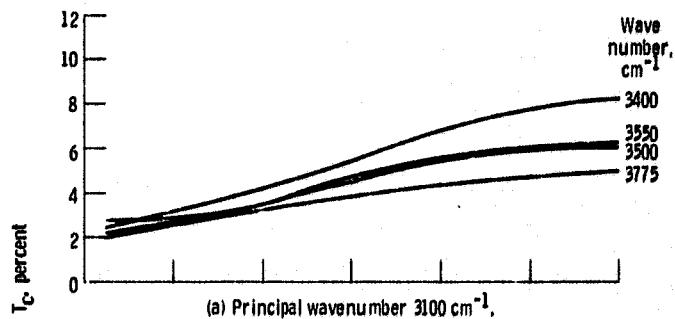


Figure 5. - Estimated error in  $T_c$  due solely to errors in radiometer and tabulated absorption coefficients. Profile of figure 1(a), with  $T_c = 2000$  K,  $T_w = 1000$  K,  $p_C = 0.35$  atm,  $p_W = 0.65$  atm,  $n_D = 0.50$ , path length 100 cm. Hydrogen-air combustion at 1 atm. Error of radiometry 1 percent, error of tabulated absorption coefficient 5 percent.

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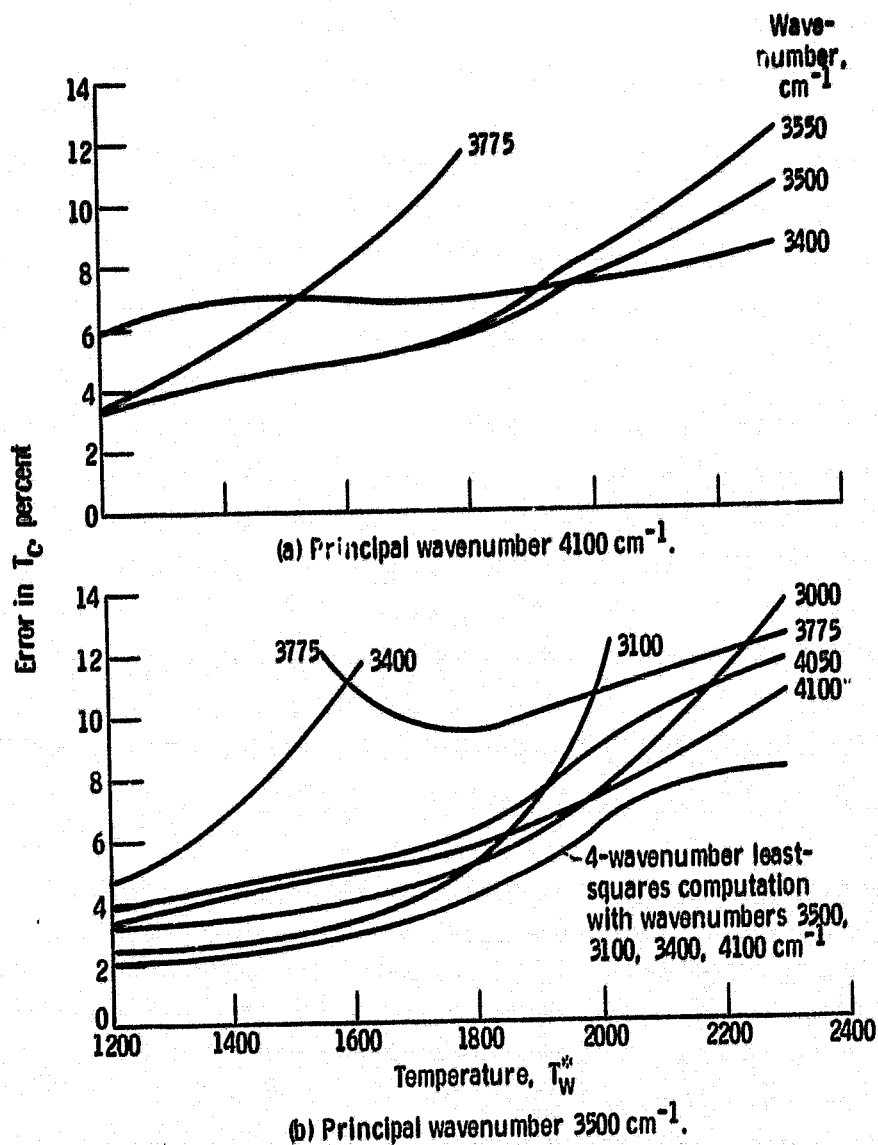


Figure 6. - Estimated error in  $T_c$  due solely to errors in radiometry and in tabulated absorption coefficients. Profile of figure 1(b) with  $T_c = 2000 \text{ K}$ ,  $n_T = 0.5$ ,  $p_c = 0.35 \text{ atm}$ ,  $p_w = 0.30 \text{ atm}$ ,  $n_p = 0.50$ , path length  $100 \text{ cm}$ . Hydrogen-air combustion at  $1 \text{ atm}$ . Error of radiometry 1 percent, tabulated absorption coefficient 5 percent.

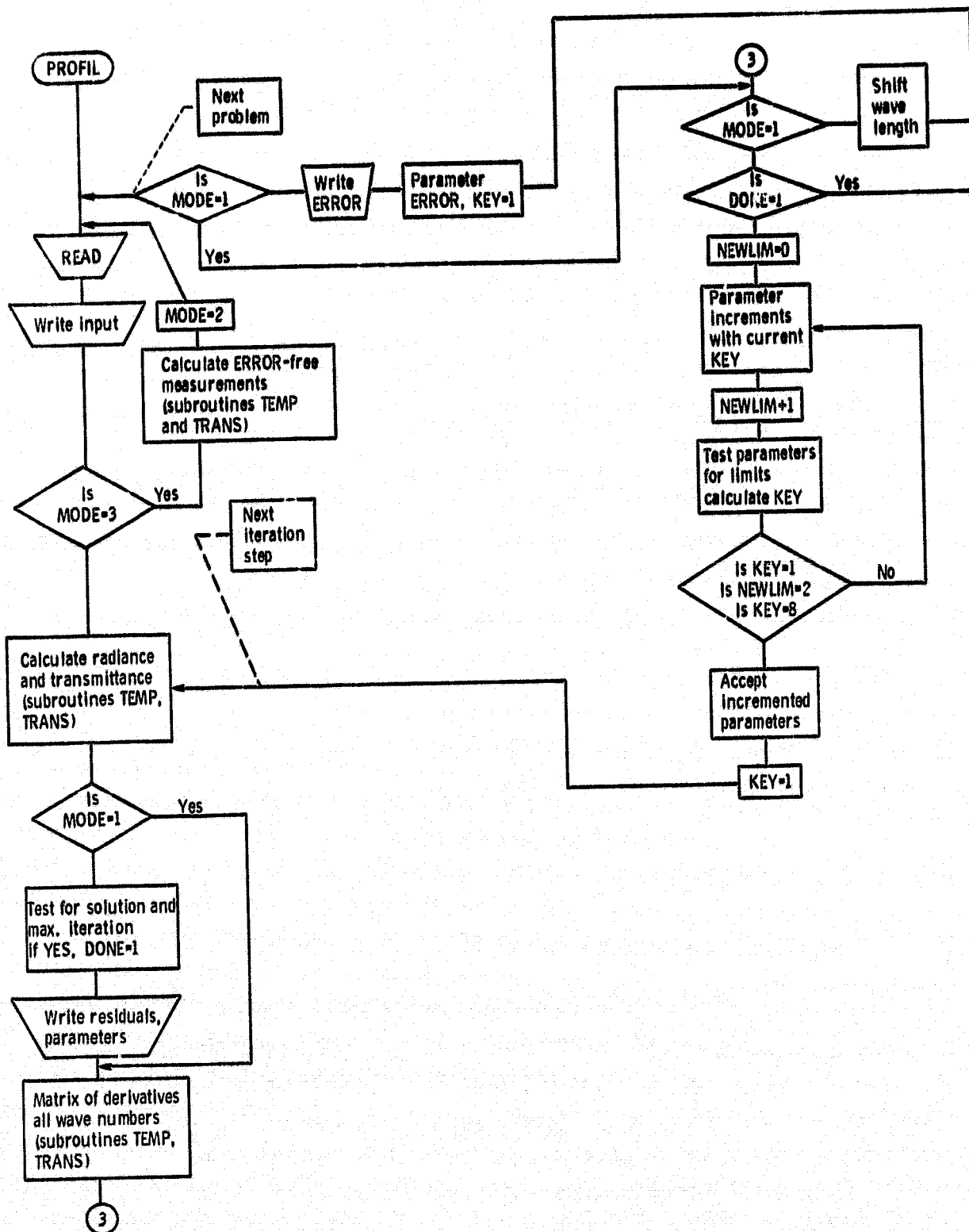


Figure 7. - Flow chart for PROFIL.

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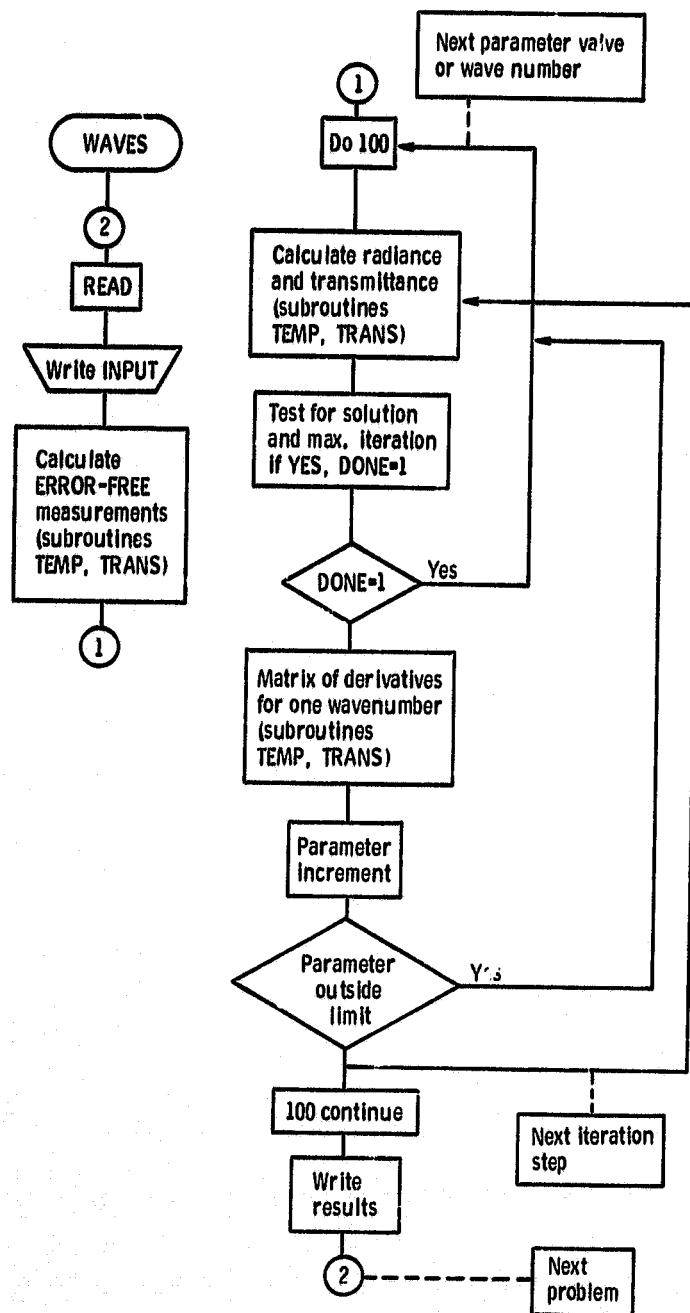
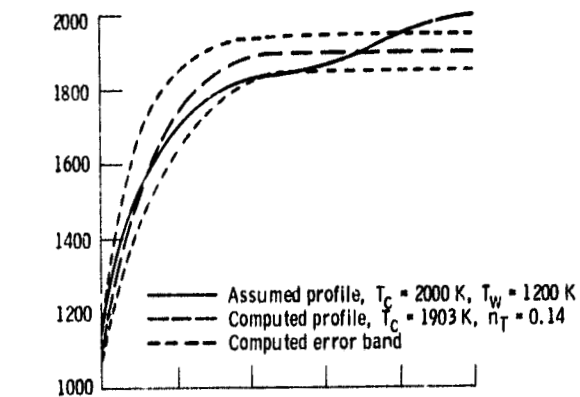
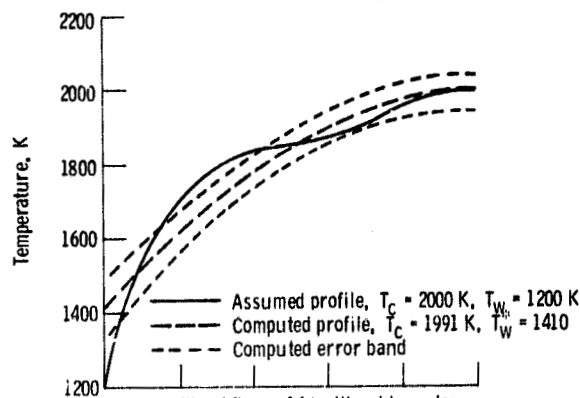


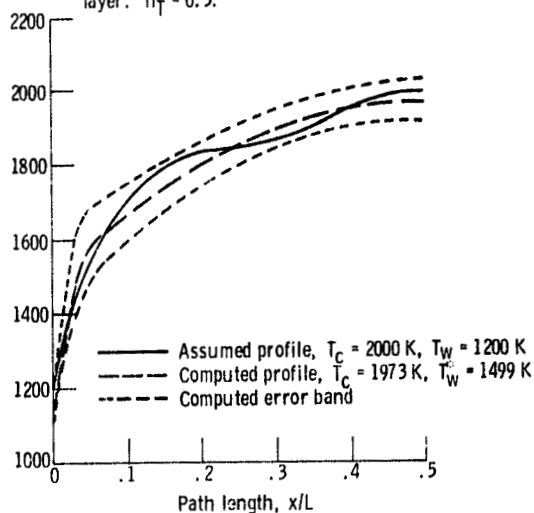
Figure 8. - Flow chart for WAVES.



(a) Profile of figure 1(a) with  $T_w = 1100$  K.



(b) Profile of figure 1(b) without boundary layer.  $n_T = 0.5$ .



(c) Profile of figure 1(b) with boundary layer.  $n_T = 0.5$ ,  $T_w = 1100$  K.

Figure 9. - Example of profile with high-temperature core. Wavenumbers of measurement  $3500$  and  $3100$   $\text{cm}^{-1}$ .

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